

Butanoic acid, 4-(2,4-dichlorophenoxy)-

Other names:

(2,4-Dichlorophenoxy)butyric acid
2,4-D butyric acid
2,4-DB
2,4-DM
4-(2,4-DB)
4-(2,4-Dichlorophenoxy)butanoic acid
4-(2,4-Dichlorophenoxy)butyric acid
Buratal
Butirex
Butormone
Butoxon
Butoxone
Butoxone ester
Butyrac
Butyrac 118
Butyrac 200
Butyrac ester
Butyric acid, 4-(2,4-dichlorophenoxy)-
Campbell's db straight
Kyselina 4-(2,4-dichlorofenoxy)maselna
Legumex
Legumex D
NSC 70337
Sys 67 Buratal
Venceweed
«gamma»-(2,4-Dichlorophenoxy)butyric acid

Inchi:

InChI=1S/C10H10Cl2O3/c11-7-3-4-9(8(12)6-7)15-5-1-2-10(13)14/h3-4,6H,1-2,5H2,(H,13)

InchiKey:

YIVXMZJTEQBQO-UHFFFAOYSA-N

Formula:

C10H10Cl2O3

SMILES:

O=C(O)CCCOc1ccc(Cl)cc1Cl

Mol. weight [g/mol]:

249.09

CAS:

94-82-6

Physical Properties

Property code	Value	Unit	Source
gf	-268.13	kJ/mol	Joback Method

hf	-464.65		kJ/mol	Joback Method
hfus	30.19		kJ/mol	Joback Method
hsub	124.00 ± 6.00		kJ/mol	NIST Webbook
hsub	149.00 ± 2.00		kJ/mol	NIST Webbook
hvap	76.06		kJ/mol	Joback Method
log10ws	-3.67			Aqueous Solubility Prediction Method
logp	3.237			Crippen Method
mcvol	165.790		ml/mol	McGowan Method
pc	3042.32		kPa	Joback Method
rinpol	1869.00			NIST Webbook
rinpol	1869.00			NIST Webbook
tb	708.17		K	Joback Method
tc	915.69		K	Joback Method
tf	391.49 ± 0.20		K	NIST Webbook
tf	390.90 ± 0.20		K	NIST Webbook
vc	0.628		m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.93	J/mol×K	881.10	Joback Method
cpg	419.62	J/mol×K	811.93	Joback Method
cpg	411.60	J/mol×K	777.34	Joback Method
cpg	402.98	J/mol×K	742.76	Joback Method
cpg	393.76	J/mol×K	708.17	Joback Method
cpg	427.06	J/mol×K	846.51	Joback Method
cpg	440.24	J/mol×K	915.69	Joback Method
dvisc	0.0009269	Paxs	446.74	Joback Method
dvisc	0.0000468	Paxs	708.17	Joback Method
dvisc	0.0000654	Paxs	664.60	Joback Method
dvisc	0.0000958	Paxs	621.03	Joback Method
dvisc	0.0001485	Paxs	577.45	Joback Method
dvisc	0.0002475	Paxs	533.88	Joback Method
dvisc	0.0004517	Paxs	490.31	Joback Method
hfust	35.00	kJ/mol	395.50	NIST Webbook
hfust	38.42	kJ/mol	391.40	NIST Webbook
hsubt	146.00 ± 1.00	kJ/mol	373.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94826&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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