

Butyric acid, 3,4-dichlorophenyl ester

Inchi:	InChI=1S/C10H10Cl2O2/c1-2-3-10(13)14-7-4-5-8(11)9(12)6-7/h4-6H,2-3H2,1H3
InchiKey:	GVUWGECOKPZWDC-UHFFFAOYSA-N
Formula:	C10H10Cl2O2
SMILES:	CCCC(=O)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	233.09

Physical Properties

Property code	Value	Unit	Source
gf	-131.31	kJ/mol	Joback Method
hf	-312.42	kJ/mol	Joback Method
hfus	26.10	kJ/mol	Joback Method
hvap	59.38	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.699		Crippen Method
mvol	159.920	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
rinpol	1569.00		NIST Webbook
tb	615.99	K	Joback Method
tc	838.92	K	Joback Method
tf	385.92	K	Joback Method
vc	0.610	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.16	J/molxK	615.99	Joback Method
cpg	360.56	J/molxK	653.15	Joback Method
cpg	371.27	J/molxK	690.30	Joback Method
cpg	381.28	J/molxK	727.46	Joback Method
cpg	390.61	J/molxK	764.61	Joback Method
cpg	399.28	J/molxK	801.77	Joback Method
cpg	407.29	J/molxK	838.92	Joback Method
dvisc	0.0012381	Paxs	385.92	Joback Method
dvisc	0.0007946	Paxs	424.26	Joback Method

dvisc	0.0005488	Paxs	462.61	Joback Method
dvisc	0.0004012	Paxs	500.96	Joback Method
dvisc	0.0003066	Paxs	539.30	Joback Method
dvisc	0.0002429	Paxs	577.64	Joback Method
dvisc	0.0001980	Paxs	615.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307517&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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