

Diethylmalonic acid, butyl 2,4-dichloro-6-formylphenyl ester

Inchi:	InChI=1S/C18H22Cl2O5/c1-4-7-8-24-16(22)18(5-2,6-3)17(23)25-15-12(11-21)9-13(19)10
InchiKey:	GQCDWRQKCLWLJV-UHFFFAOYSA-N
Formula:	C18H22Cl2O5
SMILES:	CCCCOC(=O)C(CC)(CC)C(=O)Oc1c(Cl)cc(Cl)cc1C=O
Mol. weight [g/mol]:	389.27

Physical Properties

Property code	Value	Unit	Source
gf	-404.18	kJ/mol	Joback Method
hf	-828.14	kJ/mol	Joback Method
hfus	44.09	kJ/mol	Joback Method
hvap	92.43	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	4.861		Crippen Method
mcvol	281.650	ml/mol	McGowan Method
pc	1539.08	kPa	Joback Method
rinpol	2398.00		NIST Webbook
tb	925.73	K	Joback Method
tc	1146.53	K	Joback Method
tf	605.18	K	Joback Method
vc	1.087	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.16	J/molxK	925.73	Joback Method
cpg	833.61	J/molxK	962.53	Joback Method
cpg	843.97	J/molxK	999.33	Joback Method
cpg	853.27	J/molxK	1036.13	Joback Method
cpg	861.54	J/molxK	1072.93	Joback Method
cpg	868.83	J/molxK	1109.73	Joback Method
cpg	875.16	J/molxK	1146.53	Joback Method
dvisc	0.0003230	Paxs	605.18	Joback Method
dvisc	0.0002048	Paxs	658.61	Joback Method

dvisc	0.0001391	Paxs	712.03	Joback Method
dvisc	0.0000997	Paxs	765.46	Joback Method
dvisc	0.0000746	Paxs	818.88	Joback Method
dvisc	0.0000579	Paxs	872.31	Joback Method
dvisc	0.0000462	Paxs	925.73	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370063&Units=SI

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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