

Diethylmalonic acid, 2,6-dichlorophenyl ethyl ester

Inchi:	InChI=1S/C15H18Cl2O4/c1-4-15(5-2,13(18)20-6-3)14(19)21-12-10(16)8-7-9-11(12)17/h7
InchiKey:	YFKAQOYMJVQTAH-UHFFFAOYSA-N
Formula:	C15H18Cl2O4
SMILES:	CCOC(=O)C(CC)(CC)C(=O)Oc1c(Cl)cccc1Cl
Mol. weight [g/mol]:	333.21

Physical Properties

Property code	Value	Unit	Source
gf	-320.29	kJ/mol	Joback Method
hf	-669.17	kJ/mol	Joback Method
hfus	34.42	kJ/mol	Joback Method
hvap	78.37	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.268		Crippen Method
mcvol	237.810	ml/mol	McGowan Method
pc	1857.91	kPa	Joback Method
rinsol	2026.00		NIST Webbook
tb	803.45	K	Joback Method
tc	1023.67	K	Joback Method
tf	516.85	K	Joback Method
vc	0.902	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.24	J/molxK	803.45	Joback Method
cpg	657.91	J/molxK	840.15	Joback Method
cpg	669.56	J/molxK	876.86	Joback Method
cpg	680.23	J/molxK	913.56	Joback Method
cpg	689.94	J/molxK	950.26	Joback Method
cpg	698.73	J/molxK	986.97	Joback Method
cpg	706.62	J/molxK	1023.67	Joback Method
dvisc	0.0005224	Paxs	516.85	Joback Method
dvisc	0.0003211	Paxs	564.62	Joback Method

dvisc	0.0002129	Paxs	612.38	Joback Method
dvisc	0.0001498	Paxs	660.15	Joback Method
dvisc	0.0001106	Paxs	707.92	Joback Method
dvisc	0.0000848	Paxs	755.68	Joback Method
dvisc	0.0000671	Paxs	803.45	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=U369929&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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