

Dimethylmalonic acid, 2,3-dichlorophenyl octyl ester

Inchi:	InChI=1S/C19H26Cl2O4/c1-4-5-6-7-8-9-13-24-17(22)19(2,3)18(23)25-15-12-10-11-14(20)
InchiKey:	LNYKFHVNATZGKU-UHFFFAOYSA-N
Formula:	C19H26Cl2O4
SMILES:	CCCCCCCCOC(=O)C(C)(C)C(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	389.31

Physical Properties

Property code	Value	Unit	Source
gf	-286.61	kJ/mol	Joback Method
hf	-751.73	kJ/mol	Joback Method
hfus	44.78	kJ/mol	Joback Method
hvap	87.27	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	5.829		Crippen Method
mvol	294.170	ml/mol	McGowan Method
pc	1367.69	kPa	Joback Method
rinpol	2463.00		NIST Webbook
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tb	894.97	K	Joback Method
tc	1110.14	K	Joback Method
tf	561.93	K	Joback Method
vc	1.127	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.23	J/molxK	894.97	Joback Method
cpg	884.85	J/molxK	930.83	Joback Method
cpg	897.35	J/molxK	966.69	Joback Method
cpg	908.78	J/molxK	1002.56	Joback Method
cpg	919.18	J/molxK	1038.42	Joback Method
cpg	928.59	J/molxK	1074.28	Joback Method
cpg	937.05	J/molxK	1110.14	Joback Method
dvisc	0.0003392	Paxs	561.93	Joback Method

dvisc	0.0001985	Paxs	617.44	Joback Method
dvisc	0.0001269	Paxs	672.94	Joback Method
dvisc	0.0000868	Paxs	728.45	Joback Method
dvisc	0.0000627	Paxs	783.96	Joback Method
dvisc	0.0000473	Paxs	839.46	Joback Method
dvisc	0.0000369	Paxs	894.97	Joback Method

Sources

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=U363626&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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