

Diethylmalonic acid, decyl 2,2-dichloroethyl ester

Inchi:	InChI=1S/C19H34Cl2O4/c1-4-7-8-9-10-11-12-13-14-24-17(22)19(5-2,6-3)18(23)25-15-16
InchiKey:	LUNVSCDJSHOPAF-UHFFFAOYSA-N
Formula:	C19H34Cl2O4
SMILES:	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	397.38

Physical Properties

Property code	Value	Unit	Source
gf	-382.20	kJ/mol	Joback Method
hf	-970.60	kJ/mol	Joback Method
hfus	48.00	kJ/mol	Joback Method
hvap	83.29	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.824		Crippen Method
mcvol	317.930	ml/mol	McGowan Method
pc	1113.34	kPa	Joback Method
rinsol	2311.00		NIST Webbook
tb	857.89	K	Joback Method
tc	1054.90	K	Joback Method
tf	495.47	K	Joback Method
vc	1.228	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.35	J/molxK	857.89	Joback Method
cpg	987.35	J/molxK	890.73	Joback Method
cpg	1002.29	J/molxK	923.56	Joback Method
cpg	1016.20	J/molxK	956.40	Joback Method
cpg	1029.11	J/molxK	989.23	Joback Method
cpg	1041.08	J/molxK	1022.07	Joback Method
cpg	1052.13	J/molxK	1054.90	Joback Method
dvisc	0.0006169	Paxs	495.47	Joback Method
dvisc	0.0002890	Paxs	555.87	Joback Method

dvisc	0.0001571	Paxs	616.28	Joback Method
dvisc	0.0000952	Paxs	676.68	Joback Method
dvisc	0.0000627	Paxs	737.08	Joback Method
dvisc	0.0000439	Paxs	797.49	Joback Method
dvisc	0.0000324	Paxs	857.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370785&Units=SI
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

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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