

Diethylmalonic acid, monochloride, 3,7-dimethyloctyl ester

Inchi:	InChI=1S/C17H31ClO3/c1-6-17(7-2,15(18)19)16(20)21-12-11-14(5)10-8-9-13(3)4/h13-14
InchiKey:	KFALRKOMLHREOG-UHFFFAOYSA-N
Formula:	C17H31ClO3
SMILES:	CCC(CC)(C(=O)Cl)C(=O)OCCC(C)CCCC(C)C
Mol. weight [g/mol]:	318.88

Physical Properties

Property code	Value	Unit	Source
gf	-284.55	kJ/mol	Joback Method
hf	-786.64	kJ/mol	Joback Method
hfus	33.91	kJ/mol	Joback Method
hvap	71.65	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.954		Crippen Method
mcvol	271.640	ml/mol	McGowan Method
pc	1329.07	kPa	Joback Method
rinsol	1840.00		NIST Webbook
tb	751.84	K	Joback Method
tc	942.08	K	Joback Method
tf	405.78	K	Joback Method
vc	1.044	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.33	J/molxK	751.84	Joback Method
cpg	812.26	J/molxK	783.55	Joback Method
cpg	828.21	J/molxK	815.25	Joback Method
cpg	843.23	J/molxK	846.96	Joback Method
cpg	857.34	J/molxK	878.67	Joback Method
cpg	870.60	J/molxK	910.37	Joback Method
cpg	883.03	J/molxK	942.08	Joback Method
dvisc	0.0019919	Paxs	405.78	Joback Method
dvisc	0.0007906	Paxs	463.46	Joback Method

dvisc	0.0003850	Paxs	521.13	Joback Method
dvisc	0.0002164	Paxs	578.81	Joback Method
dvisc	0.0001350	Paxs	636.49	Joback Method
dvisc	0.0000911	Paxs	694.16	Joback Method
dvisc	0.0000653	Paxs	751.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369418&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

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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