

Diethylmalonic acid, 3,7-dimethyloctyl octadecyl ester

Inchi:	InChI=1S/C35H68O4/c1-7-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-29-38-33(36)
InchiKey:	IGGJKWYVCWMTOH-UHFFFAOYSA-N
Formula:	C35H68O4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCC(C)CCCC(C)C
Mol. weight [g/mol]:	552.91

Physical Properties

Property code	Value	Unit	Source
gf	-226.06	kJ/mol	Joback Method
hf	-1274.64	kJ/mol	Joback Method
hfus	77.52	kJ/mol	Joback Method
hvap	109.74	kJ/mol	Joback Method
log10ws	-11.47		Crippen Method
logp	10.993		Crippen Method
mcvol	518.890	ml/mol	McGowan Method
pc	504.76	kPa	Joback Method
rinpol	3419.00		NIST Webbook
rinpol	3419.00		NIST Webbook
tb	1148.67	K	Joback Method
tc	1482.42	K	Joback Method
tf	600.95	K	Joback Method
vc	2.021	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1935.86	J/molxK	1148.67	Joback Method
cpg	2044.72	J/molxK	1426.79	Joback Method
cpg	2028.19	J/molxK	1371.17	Joback Method
cpg	2009.40	J/molxK	1315.54	Joback Method
cpg	1987.99	J/molxK	1259.92	Joback Method
cpg	1963.60	J/molxK	1204.29	Joback Method
cpg	2059.35	J/molxK	1482.42	Joback Method
dvisc	0.0000030	Paxs	1148.67	Joback Method

dvisc	0.0000043	Paxs	1057.38	Joback Method
dvisc	0.0000065	Paxs	966.10	Joback Method
dvisc	0.0000107	Paxs	874.81	Joback Method
dvisc	0.0000200	Paxs	783.52	Joback Method
dvisc	0.0000437	Paxs	692.24	Joback Method
dvisc	0.0001215	Paxs	600.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369416&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
mccvol:	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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