Diethylmalonic acid, di(3,7-dimethyloctyl) ester

Inchi: InChI=1S/C27H52O4/c1-9-27(10-2,25(28)30-19-17-23(7)15-11-13-21(3)4)26(29)31-20-18
InchiKey: ZJMXNGWBWASFJE-UHFFFAOYSA-N
Formula: C27H52O4
SMILES: CCC(CC)(C(=O)OCCC(C)CCCC(C)C)C(=O)OCCC(C)CCCC(C)C
Mol. weight [g/mol]: 440.70

Physical Properties

Property code	Value	Unit	Source
gf	-298.30	kJ/mol	Joback Method
hf	-1120.08	kJ/mol	Joback Method
hfus	49.75	kJ/mol	Joback Method
hvap	91.16	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	7.584		Crippen Method
mcvol	406.170	ml/mol	McGowan Method
pc	743.67	kPa	Joback Method
rinpol	2510.00		NIST Webbook
tb	964.75	K	Joback Method
tc	1183.33	K	Joback Method
tf	480.79	K	Joback Method
vc	1.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1410.69	J/mol×K	964.75	Joback Method
cpg	1431.59	J/mol×K	1001.18	Joback Method
cpg	1450.87	J/mol×K	1037.61	Joback Method
cpg	1468.59	J/mol×K	1074.04	Joback Method
cpg	1484.83	J/mol×K	1110.47	Joback Method
cpg	1499.67	J/mol×K	1146.90	Joback Method
cpg	1513.18	J/mol×K	1183.33	Joback Method
dvisc	0.0006173	Pa×s	480.79	Joback Method
dvisc	0.0001879	Pa×s	561.45	Joback Method

dvisc	0.0000771	Pa×s	642.11	Joback Method
dvisc	0.0000386	Pa×s	722.77	Joback Method
dvisc	0.0000222	Pa×s	803.43	Joback Method
dvisc	0.0000141	Pa×s	884.09	Joback Method
dvisc	0.0000097	Pa×s	964.75	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=U369417&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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