

Diethylmalonic acid, dodecyl octyl ester

Inchi: InChI=1S/C27H52O4/c1-5-9-11-13-15-16-17-18-20-22-24-31-26(29)27(7-3,8-4)25(28)30
InchiKey: GRXZESYQCUBYWTG-UHFFFAOYSA-N
Formula: C27H52O4
SMILES: CCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCCCCCC
Mol. weight [g/mol]: 440.70

Physical Properties

Property code	Value	Unit	Source
gf	-288.54	kJ/mol	Joback Method
hf	-1098.96	kJ/mol	Joback Method
hfus	63.85	kJ/mol	Joback Method
hvap	92.71	kJ/mol	Joback Method
log10ws	-8.61		Crippen Method
logp	8.161		Crippen Method
mvol	406.170	ml/mol	McGowan Method
pc	730.86	kPa	Joback Method
rinpol	2730.00		NIST Webbook
rinpol	2730.00		NIST Webbook
tb	966.51	K	Joback Method
tc	1190.06	K	Joback Method
tf	540.79	K	Joback Method
vc	1.585	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1409.34	J/molxK	966.51	Joback Method
cpg	1501.45	J/molxK	1152.80	Joback Method
cpg	1486.00	J/molxK	1115.54	Joback Method
cpg	1469.14	J/molxK	1078.28	Joback Method
cpg	1450.80	J/molxK	1041.03	Joback Method
cpg	1430.89	J/molxK	1003.77	Joback Method
cpg	1515.58	J/molxK	1190.06	Joback Method
dvisc	0.0000141	Paxs	966.51	Joback Method

dvisc	0.0000192	Paxs	895.56	Joback Method
dvisc	0.0000278	Paxs	824.60	Joback Method
dvisc	0.0000431	Paxs	753.65	Joback Method
dvisc	0.0000730	Paxs	682.70	Joback Method
dvisc	0.0001400	Paxs	611.74	Joback Method
dvisc	0.0003183	Paxs	540.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369716&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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