

Diethylmalonic acid, hept-4-yl tridecyl ester

Inchi:	InChI=1S/C27H52O4/c1-6-11-12-13-14-15-16-17-18-19-20-23-30-25(28)27(9-4,10-5)26(
InchiKey:	ACARYPUKMCCWNB-UHFFFAOYSA-N
Formula:	C27H52O4
SMILES:	CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OC(CCC)CCC
Mol. weight [g/mol]:	440.70

Physical Properties

Property code	Value	Unit	Source
gf	-290.98	kJ/mol	Joback Method
hf	-1104.24	kJ/mol	Joback Method
hfus	60.32	kJ/mol	Joback Method
hvap	92.32	kJ/mol	Joback Method
log10ws	-8.72		Crippen Method
logp	8.159		Crippen Method
mcvol	406.170	ml/mol	McGowan Method
pc	734.03	kPa	Joback Method
rinpol	2635.00		NIST Webbook
tb	966.07	K	Joback Method
tc	1188.14	K	Joback Method
tf	525.79	K	Joback Method
vc	1.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1409.68	J/molxK	966.07	Joback Method
cpg	1431.04	J/molxK	1003.08	Joback Method
cpg	1450.77	J/molxK	1040.09	Joback Method
cpg	1468.94	J/molxK	1077.10	Joback Method
cpg	1485.63	J/molxK	1114.11	Joback Method
cpg	1500.92	J/molxK	1151.12	Joback Method
cpg	1514.88	J/molxK	1188.14	Joback Method
dvisc	0.0003661	Paxs	525.79	Joback Method
dvisc	0.0001487	Paxs	599.17	Joback Method

dvisc	0.0000735	Paxs	672.55	Joback Method
dvisc	0.0000418	Paxs	745.93	Joback Method
dvisc	0.0000262	Paxs	819.31	Joback Method
dvisc	0.0000178	Paxs	892.69	Joback Method
dvisc	0.0000128	Paxs	966.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370516&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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