Diethylmalonic acid, tetradecyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C29H56O4/c1-8-11-12-13-14-15-16-17-18-19-20-21-22-32-26(30)29(9-2,10-3)
InchiKey: MGAIFHHSVBXKMT-UHFFFAOYSA-N
Formula: C29H56O4
SMILES: CCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]: 468.75

Physical Properties

Property code	Value	Unit	Source
gf	-271.30	kJ/mol	Joback Method
hf	-1154.27	kJ/mol	Joback Method
hfus	58.09	kJ/mol	Joback Method
hvap	95.48	kJ/mol	Joback Method
log10ws	-8.96		Crippen Method
logp	8.653		Crippen Method
mcvol	434.350	ml/mol	McGowan Method
pc	669.77	kPa	Joback Method
rinpol	2813.00		NIST Webbook
tb	1008.60	K	Joback Method
tc	1243.81	K	Joback Method
tf	550.75	K	Joback Method
vc	1.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1539.10	J/mol×K	1008.60	Joback Method
cpg	1561.35	J/mol×K	1047.80	Joback Method
cpg	1581.94	J/mol×K	1087.00	Joback Method
cpg	1600.99	J/mol×K	1126.21	Joback Method
cpg	1618.62	J/mol×K	1165.41	Joback Method
cpg	1634.97	J/mol×K	1204.61	Joback Method
cpg	1650.15	J/mol×K	1243.81	Joback Method
dvisc	0.0002393	Pa×s	550.75	Joback Method
dvisc	0.0000926	Pa×s	627.06	Joback Method

dvisc	0.0000440	Pa×s	703.37	Joback Method
dvisc	0.0000242	Pa×s	779.67	Joback Method
dvisc	0.0000148	Pa×s	855.98	Joback Method
dvisc	0.0000098	Pa×s	932.29	Joback Method
dvisc	0.0000069	Pa×s	1008.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369486&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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