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

Inchi: InChI=1S/C30H58O4/c1-8-11-12-13-14-15-16-17-18-19-20-21-22-23-33-27(31)30(9-2,10

InchiKey: ARLBEAMYUXWXBI-UHFFFAOYSA-N

Formula: C30H58O4

SMILES: CCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(C)CC(C)(C)C

Mol. weight [g/mol]: 482.78

Physical Properties

Property code	Value	Unit	Source
gf	-262.88	kJ/mol	Joback Method
hf	-1174.91	kJ/mol	Joback Method
hfus	60.68	kJ/mol	Joback Method
hvap	97.71	kJ/mol	Joback Method
log10ws	-9.38		Crippen Method
logp	9.043		Crippen Method
mcvol	448.440	ml/mol	McGowan Method
pc	637.69	kPa	Joback Method
rinpol	2926.00		NIST Webbook
tb	1031.48	K	Joback Method
tc	1277.17	K	Joback Method
tf	562.02	K	Joback Method
vc	1.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1604.56	J/mol×K	1031.48	Joback Method
cpg	1627.56	J/mol×K	1072.43	Joback Method
cpg	1648.77	J/mol×K	1113.38	Joback Method
cpg	1668.34	J/mol×K	1154.33	Joback Method
cpg	1686.43	J/mol×K	1195.27	Joback Method
cpg	1703.17	J/mol×K	1236.22	Joback Method
cpg	1718.73	J/mol×K	1277.17	Joback Method
dvisc	0.0002043	Pa×s	562.02	Joback Method
dvisc	0.0000786	Pa×s	640.26	Joback Method

dvisc	0.0000373	Pa×s	718.51	Joback Method
dvisc	0.0000204	Pa×s	796.75	Joback Method
dvisc	0.0000125	Pa×s	874.99	Joback Method
dvisc	0.0000083	Pa×s	953.24	Joback Method
dvisc	0.0000058	Pa×s	1031.48	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=U369487&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