Diethylmalonic acid, hexadecyl 3-methylpent-2-yl ester

Inchi: InChI=1S/C29H56O4/c1-7-11-12-13-14-15-16-17-18-19-20-21-22-23-24-32-27(30)29(9-3
InchiKey: HDYGVBSYYXIRGZ-UHFFFAOYSA-N
Formula: C29H56O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OC(C)C(C)CC
Mol. weight [g/mol]: 468.75

Physical Properties

Property code	Value	Unit	Source
gf	-276.58	kJ/mol	Joback Method
hf	-1150.80	kJ/mol	Joback Method
hfus	61.98	kJ/mol	Joback Method
hvap	96.39	kJ/mol	Joback Method
log10ws	-9.32		Crippen Method
logp	8.795		Crippen Method
mcvol	434.350	ml/mol	McGowan Method
pc	665.97	kPa	Joback Method
rinpol	2875.00		NIST Webbook
tb	1011.39	K	Joback Method
tc	1251.02	K	Joback Method
tf	533.33	K	Joback Method
vc	1.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1539.80	J/mol×K	1011.39	Joback Method
cpg	1633.79	J/mol×K	1211.08	Joback Method
cpg	1618.39	J/mol×K	1171.14	Joback Method
cpg	1601.39	J/mol×K	1131.21	Joback Method
cpg	1582.70	J/mol×K	1091.27	Joback Method
cpg	1562.21	J/mol×K	1051.33	Joback Method
cpg	1647.71	J/mol×K	1251.02	Joback Method
dvisc	0.0000084	Pa×s	1011.39	Joback Method
dvisc	0.0000118	Pa×s	931.71	Joback Method

dvisc	0.0000178	Pa×s	852.04	Joback Method
dvisc	0.0000293	Pa×s	772.36	Joback Method
dvisc	0.0000539	Pa×s	692.68	Joback Method
dvisc	0.0001161	Pa×s	613.01	Joback Method
dvisc	0.0003150	Pa×s	533.33	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U369741&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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