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

Inchi: InChI=1S/C31H60O4/c1-8-11-12-13-14-15-16-17-18-19-20-21-22-23-24-34-28(32)31(9-2

InchiKey: XZDNYJCJZUMHPF-UHFFFAOYSA-N

Formula: C31H60O4

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

Mol. weight [g/mol]: 496.81

Physical Properties

Property code	Value	Unit	Source
gf	-254.46	kJ/mol	Joback Method
hf	-1195.55	kJ/mol	Joback Method
hfus	63.27	kJ/mol	Joback Method
hvap	99.93	kJ/mol	Joback Method
log10ws	-9.80		Crippen Method
logp	9.433		Crippen Method
mcvol	462.530	ml/mol	McGowan Method
pc	607.86	kPa	Joback Method
rinpol	3033.00		NIST Webbook
tb	1054.36	K	Joback Method
tc	1311.96	K	Joback Method
tf	573.29	K	Joback Method
vc	1.792	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1670.37	J/mol×K	1054.36	Joback Method
cpg	1772.08	J/mol×K	1269.03	Joback Method
cpg	1754.87	J/mol×K	1226.10	Joback Method
cpg	1736.27	J/mol×K	1183.16	Joback Method
cpg	1716.11	J/mol×K	1140.23	Joback Method
cpg	1694.20	J/mol×K	1097.29	Joback Method
cpg	1788.08	J/mol×K	1311.96	Joback Method
dvisc	0.0000049	Pa×s	1054.36	Joback Method
dvisc	0.0000070	Pa×s	974.18	Joback Method

dvisc	0.0000105	Pa×s	894.00	Joback Method
dvisc	0.0000172	Pa×s	813.83	Joback Method
dvisc	0.0000315	Pa×s	733.65	Joback Method
dvisc	0.0000667	Pa×s	653.47	Joback Method
dvisc	0.0001741	Pa×s	573.29	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=U369488&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

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