Diethylmalonic acid, hexadecyl pentyl ester

Inchi: InChI=1S/C28H54O4/c1-5-9-11-12-13-14-15-16-17-18-19-20-21-23-25-32-27(30)28(7-3,
InchiKey: YVYGGZIJTDXRTH-UHFFFAOYSA-N
Formula: C28H54O4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCCC
Mol. weight [g/mol]: 454.73

Physical Properties

Property code	Value	Unit	Source
gf	-280.12	kJ/mol	Joback Method
hf	-1119.60	kJ/mol	Joback Method
hfus	66.44	kJ/mol	Joback Method
hvap	94.94	kJ/mol	Joback Method
log10ws	-9.03		Crippen Method
logp	8.551		Crippen Method
mcvol	420.260	ml/mol	McGowan Method
pc	694.35	kPa	Joback Method
rinpol	2868.00		NIST Webbook
rinpol	2868.00		NIST Webbook
tb	989.39	K	Joback Method
tc	1222.65	K	Joback Method
tf	552.06	K	Joback Method
vc	1.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1474.13	J/mol×K	989.39	Joback Method
cpg	1568.34	J/mol×K	1183.77	Joback Method
cpg	1552.70	J/mol×K	1144.89	Joback Method
cpg	1535.55	J/mol×K	1106.02	Joback Method
cpg	1516.80	J/mol×K	1067.14	Joback Method
cpg	1496.36	J/mol×K	1028.27	Joback Method
cpg	1582.58	J/mol×K	1222.65	Joback Method
dvisc	0.0000119	Pa×s	989.39	Joback Method

dvisc	0.0000164	Pa×s	916.50	Joback Method
dvisc	0.0000237	Pa×s	843.61	Joback Method
dvisc	0.0000368	Pa×s	770.72	Joback Method
dvisc	0.0000626	Pa×s	697.84	Joback Method
dvisc	0.0001206	Pa×s	624.95	Joback Method
dvisc	0.0002762	Pa×s	552.06	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369724&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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