Diethylmalonic acid, 2-octyl pentadecyl ester

Inchi: InChI=1S/C30H58O4/c1-6-10-12-14-15-16-17-18-19-20-21-22-24-26-33-28(31)30(8-3,9-
InchiKey: OGKWFLOYZFWVND-UHFFFAOYSA-N
Formula: C30H58O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OC(C)CCCCCC
Mol. weight [g/mol]: 482.78

Physical Properties

Property code	Value	Unit	Source
gf	-265.72	kJ/mol	Joback Method
hf	-1166.16	kJ/mol	Joback Method
hfus	68.09	kJ/mol	Joback Method
hvap	99.00	kJ/mol	Joback Method
log10ws	-9.98		Crippen Method
logp	9.329		Crippen Method
mcvol	448.440	ml/mol	McGowan Method
pc	631.61	kPa	Joback Method
rinpol	2975.00		NIST Webbook
rinpol	2975.00		NIST Webbook
tb	1034.71	K	Joback Method
tc	1288.59	K	Joback Method
tf	559.60	K	Joback Method
vc	1.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1604.99	J/mol×K	1034.71	Joback Method
cpg	1702.40	J/mol×K	1246.28	Joback Method
cpg	1686.61	J/mol×K	1203.97	Joback Method
cpg	1669.10	J/mol×K	1161.65	Joback Method
cpg	1649.75	J/mol×K	1119.34	Joback Method
cpg	1628.42	J/mol×K	1077.02	Joback Method
cpg	1716.62	J/mol×K	1288.59	Joback Method
dvisc	0.0000078	Pa×s	1034.71	Joback Method

dvisc	0.0000109	Pa×s	955.52	Joback Method
dvisc	0.0000161	Pa×s	876.34	Joback Method
dvisc	0.0000257	Pa×s	797.15	Joback Method
dvisc	0.0000457	Pa×s	717.97	Joback Method
dvisc	0.0000935	Pa×s	638.78	Joback Method
dvisc	0.0002345	Pa×s	559.60	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=U369375&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