Diethylmalonic acid, heptyl tetradecyl ester

Inchi: InChI=1S/C28H54O4/c1-5-9-11-13-14-15-16-17-18-19-21-23-25-32-27(30)28(7-3,8-4)26
InchiKey: MVHKQRQCJKPHKD-UHFFFAOYSA-N
Formula: C28H54O4
SMILES: CCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCCCCC
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	2852.00		NIST Webbook
rinpol	2852.00		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	1496.36	J/mol×K	1028.27	Joback Method
cpg	1516.80	J/mol×K	1067.14	Joback Method
cpg	1535.55	J/mol×K	1106.02	Joback Method
cpg	1552.70	J/mol×K	1144.89	Joback Method
cpg	1568.34	J/mol×K	1183.77	Joback Method
cpg	1582.58	J/mol×K	1222.65	Joback Method
dvisc	0.0002762	Pa×s	552.06	Joback Method

dvisc	0.0001206	Pa×s	624.95	Joback Method
dvisc	0.0000626	Pa×s	697.84	Joback Method
dvisc	0.0000368	Pa×s	770.72	Joback Method
dvisc	0.0000237	Pa×s	843.61	Joback Method
dvisc	0.0000164	Pa×s	916.50	Joback Method
dvisc	0.0000119	Pa×s	989.39	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=U369522&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