Diethylmalonic acid, heptadecyl 3-phenylpropyl ester

Inchi: InChI=1S/C33H56O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-23-28-36-31(34)33(5-2
InchiKey: HHPFUJUKNXNSRG-UHFFFAOYSA-N
Formula: C33H56O4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCc1ccccc1
Mol. weight [g/mol]: 516.80

Physical Properties

Property code	Value	Unit	Source
gf	-125.61	kJ/mol	Joback Method
hf	-986.27	kJ/mol	Joback Method
hfus	73.43	kJ/mol	Joback Method
hvap	108.34	kJ/mol	Joback Method
log10ws	-10.22		Crippen Method
logp	9.383		Crippen Method
mcvol	466.950	ml/mol	McGowan Method
pc	642.87	kPa	Joback Method
rinpol	3530.00		NIST Webbook
tb	1130.47	K	Joback Method
tc	1412.48	K	Joback Method
tf	634.83	K	Joback Method
vc	1.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1691.14	J/mol×K	1130.47	Joback Method
cpg	1712.22	J/mol×K	1177.47	Joback Method
cpg	1731.21	J/mol×K	1224.47	Joback Method
cpg	1748.32	J/mol×K	1271.47	Joback Method
cpg	1763.77	J/mol×K	1318.48	Joback Method
cpg	1777.78	J/mol×K	1365.48	Joback Method
cpg	1790.57	J/mol×K	1412.48	Joback Method
dvisc	0.0001142	Pa×s	634.83	Joback Method
dvisc	0.0000511	Pa×s	717.44	Joback Method

dvisc	0.0000270	Pa×s	800.04	Joback Method
dvisc	0.0000161	Pa×s	882.65	Joback Method
dvisc	0.0000105	Pa×s	965.26	Joback Method
dvisc	0.0000073	Pa×s	1047.86	Joback Method
dvisc	0.0000054	Pa×s	1130.47	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=U369667&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