Diethylmalonic acid, heptadecyl 2-isopropylphenyl ester

Inchi: InChI=1S/C33H56O4/c1-6-9-10-11-12-13-14-15-16-17-18-19-20-21-24-27-36-31(34)33(7
InchiKey: JKQWUJVRSCIAIZ-UHFFFAOYSA-N
Formula: C33H56O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1C(C)C
Mol. weight [g/mol]: 516.80

Physical Properties

Property code	Value	Unit	Source
gf	-137.68	kJ/mol	Joback Method
hf	-1003.02	kJ/mol	Joback Method
hfus	69.52	kJ/mol	Joback Method
hvap	108.62	kJ/mol	Joback Method
log10ws	-10.80		Crippen Method
logp	9.936		Crippen Method
mcvol	466.950	ml/mol	McGowan Method
pc	640.60	kPa	Joback Method
rinpol	3344.00		NIST Webbook
rinpol	3344.00		NIST Webbook
tb	1135.01	K	Joback Method
tc	1415.49	K	Joback Method
tf	632.35	K	Joback Method
vc	1.806	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1690.20	J/mol×K	1135.01	Joback Method
cpg	1710.60	J/mol×K	1181.76	Joback Method
cpg	1728.82	J/mol×K	1228.50	Joback Method
cpg	1745.08	J/mol×K	1275.25	Joback Method
cpg	1759.56	J/mol×K	1322.00	Joback Method
cpg	1772.48	J/mol×K	1368.74	Joback Method
cpg	1784.03	J/mol×K	1415.49	Joback Method
dvisc	0.0001104	Pa×s	632.35	Joback Method

dvisc	0.0000488	Pa×s	716.13	Joback Method
dvisc	0.0000256	Pa×s	799.90	Joback Method
dvisc	0.0000152	Pa×s	883.68	Joback Method
dvisc	0.0000098	Pa×s	967.46	Joback Method
dvisc	0.0000068	Pa×s	1051.23	Joback Method
dvisc	0.0000050	Pa×s	1135.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369982&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

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