Diethylmalonic acid, heptadecyl 3-methylbenzyl ester

Inchi: InChI=1S/C32H54O4/c1-5-8-9-10-11-12-13-14-15-16-17-18-19-20-21-25-35-30(33)32(6-

InchiKey: IHBIHZPYXHRFCO-UHFFFAOYSA-N

Formula: C32H54O4

SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1cccc(C)c1

Mol. weight [g/mol]: 502.77

Physical Properties

Property code	Value	Unit	Source
gf	-143.66	kJ/mol	Joback Method
hf	-977.10	kJ/mol	Joback Method
hfus	70.45	kJ/mol	Joback Method
hvap	106.78	kJ/mol	Joback Method
log10ws	-10.36		Crippen Method
logp	9.259		Crippen Method
mcvol	452.860	ml/mol	McGowan Method
pc	670.12	kPa	Joback Method
rinpol	3375.00		NIST Webbook
tb	1112.57	K	Joback Method
tc	1382.84	K	Joback Method
tf	636.08	K	Joback Method
vc	1.756	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1625.49	J/mol×K	1112.57	Joback Method
cpg	1707.47	J/mol×K	1337.80	Joback Method
cpg	1694.46	J/mol×K	1292.75	Joback Method
cpg	1679.92	J/mol×K	1247.71	Joback Method
cpg	1663.70	J/mol×K	1202.66	Joback Method
cpg	1645.62	J/mol×K	1157.62	Joback Method
cpg	1719.14	J/mol×K	1382.84	Joback Method
dvisc	0.0000065	Pa×s	1112.57	Joback Method
dvisc	0.0000088	Pa×s	1033.15	Joback Method

dvisc	0.0000124	Pa×s	953.74	Joback Method
dvisc	0.0000187	Pa×s	874.32	Joback Method
dvisc	0.0000304	Pa×s	794.91	Joback Method
dvisc	0.0000553	Pa×s	715.49	Joback Method
dvisc	0.0001168	Pa×s	636.08	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369317&Units=SI

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