Diethylmalonic acid, 2-ethylphenyl heptadecyl ester

Inchi: InChI=1S/C32H54O4/c1-5-9-10-11-12-13-14-15-16-17-18-19-20-21-24-27-35-30(33)32(7
InchiKey: QARYUTKMTGAVGM-UHFFFAOYSA-N
Formula: C32H54O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1CC
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	-10.42		Crippen Method
logp	9.375		Crippen Method
mcvol	452.860	ml/mol	McGowan Method
pc	670.12	kPa	Joback Method
rinpol	3336.00		NIST Webbook
rinpol	3336.00		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	1645.62	J/mol×K	1157.62	Joback Method
cpg	1663.70	J/mol×K	1202.66	Joback Method
cpg	1679.92	J/mol×K	1247.71	Joback Method
cpg	1694.46	J/mol×K	1292.75	Joback Method
cpg	1707.47	J/mol×K	1337.80	Joback Method
cpg	1719.14	J/mol×K	1382.84	Joback Method
dvisc	0.0001168	Pa×s	636.08	Joback Method

dvisc	0.0000553	Pa×s	715.49	Joback Method
dvisc	0.0000304	Pa×s	794.91	Joback Method
dvisc	0.0000187	Pa×s	874.32	Joback Method
dvisc	0.0000124	Pa×s	953.74	Joback Method
dvisc	0.0000088	Pa×s	1033.15	Joback Method
dvisc	0.0000065	Pa×s	1112.57	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=U370256&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