Diethylmalonic acid, pentadecyl 3-phenylpropyl ester

Inchi: InChI=1S/C31H52O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-21-26-34-29(32)31(5-2,6-3)30

InchiKey: KOPTUKVTZXFMES-UHFFFAOYSA-N

Formula: C31H52O4

SMILES: CCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCc1ccccc1

Mol. weight [g/mol]: 488.74

Physical Properties

Property code	Value	Unit	Source
gf	-142.45	kJ/mol	Joback Method
hf	-944.99	kJ/mol	Joback Method
hfus	68.25	kJ/mol	Joback Method
hvap	103.89	kJ/mol	Joback Method
log10ws	-9.39		Crippen Method
logp	8.603		Crippen Method
mcvol	438.770	ml/mol	McGowan Method
pc	710.35	kPa	Joback Method
rinpol	3309.00		NIST Webbook
tb	1084.71	K	Joback Method
tc	1341.44	K	Joback Method
tf	612.29	K	Joback Method
vc	1.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1561.76	J/mol×K	1084.71	Joback Method
cpg	1581.52	J/mol×K	1127.50	Joback Method
cpg	1599.47	J/mol×K	1170.29	Joback Method
cpg	1615.74	J/mol×K	1213.08	Joback Method
cpg	1630.49	J/mol×K	1255.86	Joback Method
cpg	1643.88	J/mol×K	1298.65	Joback Method
cpg	1656.06	J/mol×K	1341.44	Joback Method
dvisc	0.0001528	Pa×s	612.29	Joback Method
dvisc	0.0000694	Pa×s	691.03	Joback Method

dvisc	0.0000371	Pa×s	769.76	Joback Method
dvisc	0.0000222	Pa×s	848.50	Joback Method
dvisc	0.0000145	Pa×s	927.24	Joback Method
dvisc	0.0000102	Pa×s	1005.97	Joback Method
dvisc	0.0000075	Pa×s	1084.71	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369665&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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