Diethylmalonic acid, 3-chlorobenzyl hexadecyl ester

Inchi: InChI=1S/C30H49ClO4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-23-34-28(32)30(5-2,6

InchiKey: GFPJKLQNOPTAMA-UHFFFAOYSA-N

Formula: C30H49ClO4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1cccc(Cl)c1

Mol. weight [g/mol]: 509.16

Physical Properties

Property code	Value	Unit	Source
gf	-172.43	kJ/mol	Joback Method
hf	-951.56	kJ/mol	Joback Method
hfus	69.47	kJ/mol	Joback Method
hvap	106.71	kJ/mol	Joback Method
log10ws	-10.15		Crippen Method
logp	9.214		Crippen Method
mcvol	436.920	ml/mol	McGowan Method
pc	727.31	kPa	Joback Method
rinpol	3385.00		NIST Webbook
rinpol	3385.00		NIST Webbook
tb	1104.24	K	Joback Method
tc	1364.90	K	Joback Method
tf	643.46	K	Joback Method
vc	1.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1521.79	J/mol×K	1104.24	Joback Method
cpg	1539.86	J/mol×K	1147.68	Joback Method
cpg	1556.13	J/mol×K	1191.13	Joback Method
cpg	1570.77	J/mol×K	1234.57	Joback Method
cpg	1583.92	J/mol×K	1278.01	Joback Method
cpg	1595.72	J/mol×K	1321.46	Joback Method
cpg	1606.32	J/mol×K	1364.90	Joback Method
dvisc	0.0001184	Pa×s	643.46	Joback Method

dvisc	0.0000584	Pa×s	720.26	Joback Method
dvisc	0.0000330	Pa×s	797.05	Joback Method
dvisc	0.0000206	Pa×s	873.85	Joback Method
dvisc	0.0000139	Pa×s	950.65	Joback Method
dvisc	0.0000099	Pa×s	1027.44	Joback Method
dvisc	0.0000074	Pa×s	1104.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369355&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