Diethylmalonic acid, 3-chlorobenzyl dodecyl ester

Inchi: InChI=1S/C26H41ClO4/c1-4-7-8-9-10-11-12-13-14-15-19-30-24(28)26(5-2,6-3)25(29)31-

InchiKey: KDGAGAFSOJIEHT-UHFFFAOYSA-N

Formula: C26H41ClO4

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

Mol. weight [g/mol]: 453.05

Physical Properties

Property code	Value	Unit	Source
gf	-206.11	kJ/mol	Joback Method
hf	-869.00	kJ/mol	Joback Method
hfus	59.10	kJ/mol	Joback Method
hvap	97.81	kJ/mol	Joback Method
log10ws	-8.47		Crippen Method
logp	7.654		Crippen Method
mcvol	380.560	ml/mol	McGowan Method
pc	905.06	kPa	Joback Method
rinpol	2948.00		NIST Webbook
rinpol	2948.00		NIST Webbook
tb	1012.72	K	Joback Method
tc	1240.09	K	Joback Method
tf	598.38	K	Joback Method
vc	1.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1269.75	J/mol×K	1012.72	Joback Method
cpg	1286.19	J/mol×K	1050.62	Joback Method
cpg	1301.21	J/mol×K	1088.51	Joback Method
cpg	1314.90	J/mol×K	1126.41	Joback Method
cpg	1327.34	J/mol×K	1164.30	Joback Method
cpg	1338.60	J/mol×K	1202.20	Joback Method
cpg	1348.78	J/mol×K	1240.09	Joback Method
dvisc	0.0002050	Pa×s	598.38	Joback Method

dvisc	0.0001046	Pa×s	667.44	Joback Method
dvisc	0.0000606	Pa×s	736.49	Joback Method
dvisc	0.0000385	Pa×s	805.55	Joback Method
dvisc	0.0000263	Pa×s	874.61	Joback Method
dvisc	0.0000190	Pa×s	943.66	Joback Method
dvisc	0.0000144	Pa×s	1012.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369351&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