Diethylmalonic acid, 3-chlorobenzyl nonyl ester

Inchi: InChI=1S/C23H35ClO4/c1-4-7-8-9-10-11-12-16-27-21(25)23(5-2,6-3)22(26)28-18-19-14-

InchiKey: KFINDQZOISRXKY-UHFFFAOYSA-N

Formula: C23H35ClO4

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

Mol. weight [g/mol]: 410.98

Physical Properties

Property code	Value	Unit	Source
gf	-231.37	kJ/mol	Joback Method
hf	-807.08	kJ/mol	Joback Method
hfus	51.33	kJ/mol	Joback Method
hvap	91.13	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	6.483		Crippen Method
mcvol	338.290	ml/mol	McGowan Method
pc	1084.92	kPa	Joback Method
rinpol	2644.00		NIST Webbook
tb	944.08	K	Joback Method
tc	1158.58	K	Joback Method
tf	564.57	K	Joback Method
vc	1.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1085.19	J/mol×K	944.08	Joback Method
cpg	1100.85	J/mol×K	979.83	Joback Method
cpg	1115.26	J/mol×K	1015.58	Joback Method
cpg	1128.49	J/mol×K	1051.33	Joback Method
cpg	1140.58	J/mol×K	1087.08	Joback Method
cpg	1151.60	J/mol×K	1122.83	Joback Method
cpg	1161.61	J/mol×K	1158.58	Joback Method
dvisc	0.0003023	Pa×s	564.57	Joback Method
dvisc	0.0001588	Pa×s	627.82	Joback Method

dvisc	0.0000939	Pa×s	691.07	Joback Method
dvisc	0.0000606	Pa×s	754.32	Joback Method
dvisc	0.0000419	Pa×s	817.58	Joback Method
dvisc	0.0000305	Pa×s	880.83	Joback Method
dvisc	0.0000232	Pa×s	944.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369349&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