

Diethylmalonic acid, 4-chlorobenzyl nonyl ester

Inchi:	InChI=1S/C23H35ClO4/c1-4-7-8-9-10-11-12-17-27-21(25)23(5-2,6-3)22(26)28-18-19-13
InchiKey:	UWIMXZHKZXJGFW-UHFFFAOYSA-N
Formula:	C23H35ClO4
SMILES:	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1ccc(Cl)cc1
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	2651.00		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/molxK	944.08	Joback Method
cpg	1100.85	J/molxK	979.83	Joback Method
cpg	1115.26	J/molxK	1015.58	Joback Method
cpg	1128.49	J/molxK	1051.33	Joback Method
cpg	1140.58	J/molxK	1087.08	Joback Method
cpg	1151.60	J/molxK	1122.83	Joback Method
cpg	1161.61	J/molxK	1158.58	Joback Method
dvisc	0.0003023	Paxs	564.57	Joback Method
dvisc	0.0001588	Paxs	627.82	Joback Method

dvisc	0.0000939	Paxs	691.07	Joback Method
dvisc	0.0000606	Paxs	754.32	Joback Method
dvisc	0.0000419	Paxs	817.58	Joback Method
dvisc	0.0000305	Paxs	880.83	Joback Method
dvisc	0.0000232	Paxs	944.08	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=U369781&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

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