

Diethylmalonic acid, 2-chloro-5-methylphenyl nonyl ester

Inchi:	InChI=1S/C23H35ClO4/c1-5-8-9-10-11-12-13-16-27-21(25)23(6-2,7-3)22(26)28-20-17-18
InchiKey:	NCYGPRGBVFBWRO-UHFFFAOYSA-N
Formula:	C23H35ClO4
SMILES:	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cc(C)ccc1Cl
Mol. weight [g/mol]:	410.98

Physical Properties

Property code	Value	Unit	Source
gf	-241.00	kJ/mol	Joback Method
hf	-818.55	kJ/mol	Joback Method
hfus	50.95	kJ/mol	Joback Method
hvap	91.79	kJ/mol	Joback Method
log10ws	-7.43		Crippen Method
logp	6.654		Crippen Method
mcvol	338.290	ml/mol	McGowan Method
pc	1074.28	kPa	Joback Method
rinpol	2622.00		NIST Webbook
tb	949.06	K	Joback Method
tc	1164.53	K	Joback Method
tf	577.09	K	Joback Method
vc	1.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1084.39	J/molxK	949.06	Joback Method
cpg	1099.96	J/molxK	984.97	Joback Method
cpg	1114.25	J/molxK	1020.88	Joback Method
cpg	1127.33	J/molxK	1056.79	Joback Method
cpg	1139.25	J/molxK	1092.70	Joback Method
cpg	1150.06	J/molxK	1128.62	Joback Method
cpg	1159.81	J/molxK	1164.53	Joback Method
dvisc	0.0002646	Paxs	577.09	Joback Method
dvisc	0.0001455	Paxs	639.08	Joback Method

dvisc	0.0000890	Paxs	701.08	Joback Method
dvisc	0.0000589	Paxs	763.07	Joback Method
dvisc	0.0000415	Paxs	825.07	Joback Method
dvisc	0.0000307	Paxs	887.06	Joback Method
dvisc	0.0000236	Paxs	949.06	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=U370459&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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