Diethylmalonic acid, 4-chloro-3-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)28-19-14-15

InchiKey: NFBMWIHOBYEOSN-UHFFFAOYSA-N

Formula: C23H35ClO4

SMILES: CCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Cl)c(C)c1

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	2627.00		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/mol×K	949.06	Joback Method
cpg	1150.06	J/mol×K	1128.62	Joback Method
cpg	1139.25	J/mol×K	1092.70	Joback Method
cpg	1127.33	J/mol×K	1056.79	Joback Method
cpg	1114.25	J/mol×K	1020.88	Joback Method
cpg	1099.96	J/mol×K	984.97	Joback Method
cpg	1159.81	J/mol×K	1164.53	Joback Method
dvisc	0.0000236	Pa×s	949.06	Joback Method
dvisc	0.0000307	Pa×s	887.06	Joback Method

dvisc	0.0000415	Pa×s	825.07	Joback Method
dvisc	0.0000589	Pa×s	763.07	Joback Method
dvisc	0.0000890	Pa×s	701.08	Joback Method
dvisc	0.0001455	Pa×s	639.08	Joback Method
dvisc	0.0002646	Pa×s	577.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369918&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

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