Dimethylmalonic acid, 2,3-dichlorophenyl nonyl ester

Inchi: InChI=1S/C20H28Cl2O4/c1-4-5-6-7-8-9-10-14-25-18(23)20(2,3)19(24)26-16-13-11-12-15

InchiKey: OVJQUUPCLMNZPL-UHFFFAOYSA-N

Formula: C20H28Cl2O4

SMILES: CCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 403.34

Physical Properties

Property code	Value	Unit	Source
gf	-278.19	kJ/mol	Joback Method
hf	-772.37	kJ/mol	Joback Method
hfus	47.37	kJ/mol	Joback Method
hvap	89.50	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	6.219		Crippen Method
mcvol	308.260	ml/mol	McGowan Method
pc	1275.51	kPa	Joback Method
rinpol	2563.00		NIST Webbook
tb	917.85	K	Joback Method
tc	1133.54	K	Joback Method
tf	573.20	K	Joback Method
vc	1.183	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	929.71	J/mol×K	917.85	Joback Method
cpg	987.76	J/mol×K	1097.60	Joback Method
cpg	978.25	J/mol×K	1061.65	Joback Method
cpg	967.74	J/mol×K	1025.70	Joback Method
cpg	956.18	J/mol×K	989.75	Joback Method
cpg	943.52	J/mol×K	953.80	Joback Method
cpg	996.30	J/mol×K	1133.54	Joback Method
dvisc	0.0000316	Pa×s	917.85	Joback Method
dvisc	0.0000406	Pa×s	860.41	Joback Method

dvisc	0.0000541	Pa×s	802.97	Joback Method
dvisc	0.0000753	Pa×s	745.52	Joback Method
dvisc	0.0001107	Pa×s	688.08	Joback Method
dvisc	0.0001747	Pa×s	630.64	Joback Method
dvisc	0.0003019	Pa×s	573.20	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=U363627&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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