

Dimethylmalonic acid, 2,5-dichlorophenyl nonyl ester

Inchi:	InChI=1S/C20H28Cl2O4/c1-4-5-6-7-8-9-10-13-25-18(23)20(2,3)19(24)26-17-14-15(21)1
InchiKey:	JJXVYNCDJSXWEW-UHFFFAOYSA-N
Formula:	C20H28Cl2O4
SMILES:	CCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1cc(Cl)ccc1Cl
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
rinsol	2509.00		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/molxK	917.85	Joback Method
cpg	943.52	J/molxK	953.80	Joback Method
cpg	956.18	J/molxK	989.75	Joback Method
cpg	967.74	J/molxK	1025.70	Joback Method
cpg	978.25	J/molxK	1061.65	Joback Method
cpg	987.76	J/molxK	1097.60	Joback Method
cpg	996.30	J/molxK	1133.54	Joback Method
dvisc	0.0003019	Paxs	573.20	Joback Method
dvisc	0.0001747	Paxs	630.64	Joback Method

dvisc	0.0001107	Paxs	688.08	Joback Method
dvisc	0.0000753	Paxs	745.52	Joback Method
dvisc	0.0000541	Paxs	802.97	Joback Method
dvisc	0.0000406	Paxs	860.41	Joback Method
dvisc	0.0000316	Paxs	917.85	Joback Method

Sources

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=U363686&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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