

Diethylmalonic acid, 3,5-dichlorophenyl nonyl ester

Inchi:	InChI=1S/C22H32Cl2O4/c1-4-7-8-9-10-11-12-13-27-20(25)22(5-2,6-3)21(26)28-19-15-17
InchiKey:	WDLGUNVIHFYIKR-UHFFFAOYSA-N
Formula:	C22H32Cl2O4
SMILES:	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]:	431.39

Physical Properties

Property code	Value	Unit	Source
gf	-261.35	kJ/mol	Joback Method
hf	-813.65	kJ/mol	Joback Method
hfus	52.55	kJ/mol	Joback Method
hvap	93.95	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	6.999		Crippen Method
mcvol	336.440	ml/mol	McGowan Method
pc	1117.06	kPa	Joback Method
rinpol	2634.00		NIST Webbook
rinpol	2634.00		NIST Webbook
tb	963.61	K	Joback Method
tc	1182.85	K	Joback Method
tf	595.74	K	Joback Method
vc	1.294	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1048.62	J/molxK	963.61	Joback Method
cpg	1062.83	J/molxK	1000.15	Joback Method
cpg	1075.81	J/molxK	1036.69	Joback Method
cpg	1087.62	J/molxK	1073.23	Joback Method
cpg	1098.32	J/molxK	1109.77	Joback Method
cpg	1107.97	J/molxK	1146.31	Joback Method
cpg	1116.62	J/molxK	1182.85	Joback Method
dvisc	0.0002370	Paxs	595.74	Joback Method

dvisc	0.0001342	Paxs	657.05	Joback Method
dvisc	0.0000837	Paxs	718.36	Joback Method
dvisc	0.0000562	Paxs	779.67	Joback Method
dvisc	0.0000400	Paxs	840.99	Joback Method
dvisc	0.0000299	Paxs	902.30	Joback Method
dvisc	0.0000231	Paxs	963.61	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=U370443&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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