

Diethylmalonic acid, octyl 2,3,5-trichlorophenyl ester

Inchi:	InChI=1S/C21H29Cl3O4/c1-4-7-8-9-10-11-12-27-19(25)21(5-2,6-3)20(26)28-17-14-15(22)
InchiKey:	CRACSYLLJSKESK-UHFFFAOYSA-N
Formula:	C21H29Cl3O4
SMILES:	CCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cc(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]:	451.81

Physical Properties

Property code	Value	Unit	Source
gf	-291.33	kJ/mol	Joback Method
hf	-820.22	kJ/mol	Joback Method
hfus	53.77	kJ/mol	Joback Method
hvap	96.77	kJ/mol	Joback Method
log10ws	-7.90		Crippen Method
logp	7.262		Crippen Method
mvol	334.590	ml/mol	McGowan Method
pc	1150.65	kPa	Joback Method
rinpol	2709.00		NIST Webbook
rinpol	2709.00		NIST Webbook
tb	983.14	K	Joback Method
tc	1207.14	K	Joback Method
tf	626.91	K	Joback Method
vc	1.288	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1010.50	J/molxK	983.14	Joback Method
cpg	1062.73	J/molxK	1169.81	Joback Method
cpg	1054.48	J/molxK	1132.48	Joback Method
cpg	1045.18	J/molxK	1095.14	Joback Method
cpg	1034.79	J/molxK	1057.81	Joback Method
cpg	1023.25	J/molxK	1020.47	Joback Method
cpg	1069.97	J/molxK	1207.14	Joback Method
dvisc	0.0000230	Paxs	983.14	Joback Method

dvisc	0.0000293	Paxs	923.77	Joback Method
dvisc	0.0000384	Paxs	864.40	Joback Method
dvisc	0.0000525	Paxs	805.02	Joback Method
dvisc	0.0000754	Paxs	745.65	Joback Method
dvisc	0.0001152	Paxs	686.28	Joback Method
dvisc	0.0001909	Paxs	626.91	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=U370550&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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