

Diethylmalonic acid, 3,5-dichlorophenyl pentyl ester

Inchi:	InChI=1S/C18H24Cl2O4/c1-4-7-8-9-23-16(21)18(5-2,6-3)17(22)24-15-11-13(19)10-14(20)
InchiKey:	QIYIIHDRVNPUBC-UHFFFAOYSA-N
Formula:	C18H24Cl2O4
SMILES:	CCCCCOC(=O)C(CC)(CC)C(=O)Oc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]:	375.29

Physical Properties

Property code	Value	Unit	Source
gf	-295.03	kJ/mol	Joback Method
hf	-731.09	kJ/mol	Joback Method
hfus	42.19	kJ/mol	Joback Method
hvap	85.05	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	5.439		Crippen Method
mcvol	280.080	ml/mol	McGowan Method
pc	1470.23	kPa	Joback Method
rinpol	2253.00		NIST Webbook
tb	872.09	K	Joback Method
tc	1087.50	K	Joback Method
tf	550.66	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.48	J/molxK	872.09	Joback Method
cpg	826.90	J/molxK	907.99	Joback Method
cpg	839.23	J/molxK	943.89	Joback Method
cpg	850.50	J/molxK	979.79	Joback Method
cpg	860.77	J/molxK	1015.70	Joback Method
cpg	870.07	J/molxK	1051.60	Joback Method
cpg	878.44	J/molxK	1087.50	Joback Method
dvisc	0.0003800	Paxs	550.66	Joback Method
dvisc	0.0002249	Paxs	604.23	Joback Method

dvisc	0.0001450	Paxs	657.80	Joback Method
dvisc	0.0000999	Paxs	711.38	Joback Method
dvisc	0.0000725	Paxs	764.95	Joback Method
dvisc	0.0000549	Paxs	818.52	Joback Method
dvisc	0.0000430	Paxs	872.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370439&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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