

Diethylmalonic acid, monochloride, 2,4-dichloronaphth-1-yl ester

Inchi:	InChI=1S/C17H15Cl3O3/c1-3-17(4-2,15(20)21)16(22)23-14-11-8-6-5-7-10(11)12(18)9-13
InchiKey:	KSMRWOOMQXDVRA-UHFFFAOYSA-N
Formula:	C17H15Cl3O3
SMILES:	CCC(CC)(C(=O)Cl)C(=O)Oc1c(Cl)cc(Cl)c2ccccc12
Mol. weight [g/mol]:	373.66

Physical Properties

Property code	Value	Unit	Source
gf	-113.36	kJ/mol	Joback Method
hf	-414.37	kJ/mol	Joback Method
hfus	39.24	kJ/mol	Joback Method
hvap	87.10	kJ/mol	Joback Method
log10ws	-6.74		Crippen Method
logp	5.624		Crippen Method
mcvol	252.900	ml/mol	McGowan Method
pc	1887.08	kPa	Joback Method
rinpol	2598.00		NIST Webbook
tb	888.18	K	Joback Method
tc	1128.74	K	Joback Method
tf	592.30	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.46	J/molxK	888.18	Joback Method
cpg	683.33	J/molxK	928.27	Joback Method
cpg	693.37	J/molxK	968.37	Joback Method
cpg	702.67	J/molxK	1008.46	Joback Method
cpg	711.33	J/molxK	1048.55	Joback Method
cpg	719.44	J/molxK	1088.65	Joback Method
cpg	727.11	J/molxK	1128.74	Joback Method
dvisc	0.0005795	Paxs	592.30	Joback Method
dvisc	0.0003997	Paxs	641.61	Joback Method

dvisc	0.0002907	Paxs	690.93	Joback Method
dvisc	0.0002206	Paxs	740.24	Joback Method
dvisc	0.0001733	Paxs	789.55	Joback Method
dvisc	0.0001400	Paxs	838.87	Joback Method
dvisc	0.0001159	Paxs	888.18	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=U370060&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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