Diethylmalonic acid, monochloride, 2-naphthylmethyl ester

Inchi: InChI=1S/C18H19ClO3/c1-3-18(4-2,16(19)20)17(21)22-12-13-9-10-14-7-5-6-8-15(14)11-

InchiKey: IOYZUTNBQPUOLE-UHFFFAOYSA-N

Formula: C18H19ClO3

SMILES: CCC(CC)(C(=O)Cl)C(=O)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 318.80

Physical Properties

Property code	Value	Unit	Source
gf	-61.82	kJ/mol	Joback Method
hf	-380.59	kJ/mol	Joback Method
hfus	34.22	kJ/mol	Joback Method
hvap	79.23	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	4.455		Crippen Method
mcvol	242.510	ml/mol	McGowan Method
pc	1900.26	kPa	Joback Method
rinpol	2352.00		NIST Webbook
tb	826.24	K	Joback Method
tc	1056.94	K	Joback Method
tf	518.69	K	Joback Method
vc	0.925	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	687.93	J/mol×K	826.24	Joback Method
cpg	701.50	J/mol×K	864.69	Joback Method
cpg	714.06	J/mol×K	903.14	Joback Method
cpg	725.71	J/mol×K	941.59	Joback Method
cpg	736.55	J/mol×K	980.04	Joback Method
cpg	746.69	J/mol×K	1018.49	Joback Method
cpg	756.21	J/mol×K	1056.94	Joback Method
dvisc	0.0009058	Pa×s	518.69	Joback Method
dvisc	0.0005656	Pa×s	569.95	Joback Method

dvisc	0.0003817	Pa×s	621.21	Joback Method
dvisc	0.0002735	Pa×s	672.47	Joback Method
dvisc	0.0002055	Pa×s	723.72	Joback Method
dvisc	0.0001603	Pa×s	774.98	Joback Method
dvisc	0.0001290	Pa×s	826.24	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=U370560&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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