

Diethylmalonic acid, di(4-chloro-2-methylphenyl) ester

Inchi: InChI=1S/C21H22Cl2O4/c1-5-21(6-2,19(24)26-17-9-7-15(22)11-13(17)3)20(25)27-18-10

InchiKey: SODKJMQSWWNUEH-UHFFFAOYSA-N

Formula: C21H22Cl2O4

SMILES: CCC(CC)(C(=O)Oc1ccc(Cl)cc1C)C(=O)Oc1ccc(Cl)cc1C

Mol. weight [g/mol]: 409.30

Physical Properties

Property code	Value	Unit	Source
gf	-176.62	kJ/mol	Joback Method
hf	-579.42	kJ/mol	Joback Method
hfus	43.23	kJ/mol	Joback Method
hvap	95.33	kJ/mol	Joback Method
log10ws	-7.08		Crippen Method
logp	5.928		Crippen Method
mvol	298.590	ml/mol	McGowan Method
pc	1485.00	kPa	Joback Method
rinpol	2791.00		NIST Webbook
rinpol	2791.00		NIST Webbook
tb	977.37	K	Joback Method
tc	1216.62	K	Joback Method
tf	635.93	K	Joback Method
vc	1.131	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.91	J/molxK	977.37	Joback Method
cpg	891.37	J/molxK	1017.24	Joback Method
cpg	901.54	J/molxK	1057.12	Joback Method
cpg	910.50	J/molxK	1096.99	Joback Method
cpg	918.30	J/molxK	1136.87	Joback Method
cpg	925.00	J/molxK	1176.74	Joback Method
cpg	930.65	J/molxK	1216.62	Joback Method
dvisc	0.0001957	Paxs	635.93	Joback Method

dvisc	0.0001250	Paxs	692.84	Joback Method
dvisc	0.0000855	Paxs	749.74	Joback Method
dvisc	0.0000617	Paxs	806.65	Joback Method
dvisc	0.0000465	Paxs	863.56	Joback Method
dvisc	0.0000362	Paxs	920.46	Joback Method
dvisc	0.0000291	Paxs	977.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370122&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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