Diethylmalonic acid, di(2-chloro-5-methylphenyl) ester

Inchi: InChI=1S/C21H22Cl2O4/c1-5-21(6-2,19(24)26-17-11-13(3)7-9-15(17)22)20(25)27-18-12

InchiKey: RNHLPQNXBVSPCF-UHFFFAOYSA-N

Formula: C21H22Cl2O4

SMILES: CCC(CC)(C(=O)Oc1cc(C)ccc1Cl)C(=O)Oc1cc(C)ccc1Cl

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
mcvol	298.590	ml/mol	McGowan Method
pc	1485.00	kPa	Joback Method
rinpol	2719.00		NIST Webbook
tb	977.37	K	Joback Method
tc	1216.62	K	Joback Method
tf	635.93	K	Joback Method
vc	1.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.91	J/mol×K	977.37	Joback Method
cpg	891.37	J/mol×K	1017.24	Joback Method
cpg	901.54	J/mol×K	1057.12	Joback Method
cpg	910.50	J/mol×K	1096.99	Joback Method
cpg	918.30	J/mol×K	1136.87	Joback Method
cpg	925.00	J/mol×K	1176.74	Joback Method
cpg	930.65	J/mol×K	1216.62	Joback Method
dvisc	0.0001957	Pa×s	635.93	Joback Method
dvisc	0.0001250	Pa×s	692.84	Joback Method

dvisc	0.0000855	Pa×s	749.74	Joback Method
dvisc	0.0000617	Pa×s	806.65	Joback Method
dvisc	0.0000465	Pa×s	863.56	Joback Method
dvisc	0.0000362	Pa×s	920.46	Joback Method
dvisc	0.0000291	Pa×s	977.37	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U370467&Units=SI

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