Diethylmalonic acid, di(2,4-dichlorophenyl) ester

Inchi: InChI=1S/C19H16Cl4O4/c1-3-19(4-2,17(24)26-15-7-5-11(20)9-13(15)22)18(25)27-16-8-6-
InchiKey: CZSSAJXJLWZZTC-UHFFFAOYSA-N
Formula: C19H16Cl4O4
SMILES: CCC(CC)(C(=O)Oc1ccc(Cl)cc1Cl)C(=O)Oc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 450.14

Physical Properties

Property code	Value	Unit	Source
gf	-217.32	kJ/mol	Joback Method
hf	-569.62	kJ/mol	Joback Method
hfus	46.44	kJ/mol	Joback Method
hvap	99.64	kJ/mol	Joback Method
log10ws	-7.50		Crippen Method
logp	6.618		Crippen Method
mcvol	294.890	ml/mol	McGowan Method
pc	1629.85	kPa	Joback Method
rinpol	2911.00		NIST Webbook
rinpol	2911.00		NIST Webbook
tb	1006.47	K	Joback Method
tc	1255.53	K	Joback Method
tf	673.23	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	801.39	J/mol×K	1006.47	Joback Method
cpg	810.02	J/mol×K	1047.98	Joback Method
cpg	817.49	J/mol×K	1089.49	Joback Method
cpg	823.86	J/mol×K	1131.00	Joback Method
cpg	829.20	J/mol×K	1172.51	Joback Method
cpg	833.56	J/mol×K	1214.02	Joback Method
cpg	837.01	J/mol×K	1255.53	Joback Method
dvisc	0.0001654	Pa×s	673.23	Joback Method

dvisc	0.0001098	Pa×s	728.77	Joback Method
dvisc	0.0000772	Pa×s	784.31	Joback Method
dvisc	0.0000569	Pa×s	839.85	Joback Method
dvisc	0.0000435	Pa×s	895.39	Joback Method
dvisc	0.0000344	Pa×s	950.93	Joback Method
dvisc	0.0000278	Pa×s	1006.47	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=U369579&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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