

Diethylmalonic acid, 2,4-dichloro-6-formylphenyl heptyl ester

Inchi:	InChI=1S/C21H28Cl2O5/c1-4-7-8-9-10-11-27-19(25)21(5-2,6-3)20(26)28-18-15(14-24)12
InchiKey:	HCHSNWRZMJCMDW-UHFFFAOYSA-N
Formula:	C21H28Cl2O5
SMILES:	CCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(Cl)cc(Cl)cc1C=O
Mol. weight [g/mol]:	431.35

Physical Properties

Property code	Value	Unit	Source
gf	-378.92	kJ/mol	Joback Method
hf	-890.06	kJ/mol	Joback Method
hfus	51.86	kJ/mol	Joback Method
hvap	99.11	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	6.031		Crippen Method
mvol	323.920	ml/mol	McGowan Method
pc	1242.46	kPa	Joback Method
rinpol	2684.00		NIST Webbook
rinpol	2684.00		NIST Webbook
tb	994.37	K	Joback Method
tc	1219.80	K	Joback Method
tf	638.99	K	Joback Method
vc	1.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.03	J/molxK	994.37	Joback Method
cpg	1009.07	J/molxK	1031.94	Joback Method
cpg	1019.90	J/molxK	1069.51	Joback Method
cpg	1029.55	J/molxK	1107.09	Joback Method
cpg	1038.07	J/molxK	1144.66	Joback Method
cpg	1045.52	J/molxK	1182.23	Joback Method
cpg	1051.95	J/molxK	1219.80	Joback Method
dvisc	0.0002277	Paxs	638.99	Joback Method

dvisc	0.0001397	Paxs	698.22	Joback Method
dvisc	0.0000925	Paxs	757.45	Joback Method
dvisc	0.0000651	Paxs	816.68	Joback Method
dvisc	0.0000480	Paxs	875.91	Joback Method
dvisc	0.0000368	Paxs	935.14	Joback Method
dvisc	0.0000291	Paxs	994.37	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370067&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

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