

Diethylmalonic acid, heptyl 2,4,5-trichlorophenyl ester

Inchi:	InChI=1S/C20H27Cl3O4/c1-4-7-8-9-10-11-26-18(24)20(5-2,6-3)19(25)27-17-13-15(22)14
InchiKey:	PMHFRXGFCIAZNW-UHFFFAOYSA-N
Formula:	C20H27Cl3O4
SMILES:	CCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	437.79

Physical Properties

Property code	Value	Unit	Source
gf	-299.75	kJ/mol	Joback Method
hf	-799.58	kJ/mol	Joback Method
hfus	51.18	kJ/mol	Joback Method
hvap	94.55	kJ/mol	Joback Method
log10ws	-7.48		Crippen Method
logp	6.872		Crippen Method
mvol	320.500	ml/mol	McGowan Method
pc	1229.42	kPa	Joback Method
rinpol	2638.00		NIST Webbook
rinpol	2638.00		NIST Webbook
tb	960.26	K	Joback Method
tc	1182.24	K	Joback Method
tf	615.64	K	Joback Method
vc	1.232	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	951.39	J/molxK	960.26	Joback Method
cpg	963.93	J/molxK	997.26	Joback Method
cpg	975.32	J/molxK	1034.25	Joback Method
cpg	985.60	J/molxK	1071.25	Joback Method
cpg	994.81	J/molxK	1108.25	Joback Method
cpg	1003.00	J/molxK	1145.24	Joback Method
cpg	1010.21	J/molxK	1182.24	Joback Method
dvisc	0.0002155	Paxs	615.64	Joback Method

dvisc	0.0001315	Paxs	673.08	Joback Method
dvisc	0.0000867	Paxs	730.51	Joback Method
dvisc	0.0000608	Paxs	787.95	Joback Method
dvisc	0.0000447	Paxs	845.39	Joback Method
dvisc	0.0000342	Paxs	902.82	Joback Method
dvisc	0.0000270	Paxs	960.26	Joback Method

Sources

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=U370534&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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