

Sebacic acid, ethyl 2,3,6-trichlorophenyl ester

Inchi:	InChI=1S/C18H23Cl3O4/c1-2-24-15(22)9-7-5-3-4-6-8-10-16(23)25-18-14(20)12-11-13(19)
InchiKey:	VOOCMHFBHDJDEZ-UHFFFAOYSA-N
Formula:	C18H23Cl3O4
SMILES:	CCOC(=O)CCCCCCCC(=O)Oc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]:	409.73

Physical Properties

Property code	Value	Unit	Source
gf	-319.43	kJ/mol	Joback Method
hf	-749.55	kJ/mol	Joback Method
hfus	53.41	kJ/mol	Joback Method
hvap	91.39	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	6.236		Crippen Method
mcvol	292.320	ml/mol	McGowan Method
pc	1393.33	kPa	Joback Method
rinqol	2798.00		NIST Webbook
tb	917.73	K	Joback Method
tc	1133.26	K	Joback Method
tf	590.68	K	Joback Method
vc	1.131	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	834.27	J/molxK	917.73	Joback Method
cpg	883.34	J/molxK	1097.33	Joback Method
cpg	875.72	J/molxK	1061.41	Joback Method
cpg	867.01	J/molxK	1025.49	Joback Method
cpg	857.21	J/molxK	989.57	Joback Method
cpg	846.30	J/molxK	953.65	Joback Method
cpg	889.90	J/molxK	1133.26	Joback Method
dvisc	0.0000477	Paxs	917.73	Joback Method
dvisc	0.0000592	Paxs	863.22	Joback Method

dvisc	0.0000757	Paxs	808.71	Joback Method
dvisc	0.0001001	Paxs	754.21	Joback Method
dvisc	0.0001384	Paxs	699.70	Joback Method
dvisc	0.0002021	Paxs	645.19	Joback Method
dvisc	0.0003165	Paxs	590.68	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=U355259&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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