

Sebacic acid, propyl 3,4,5-trichlorophenyl ester

Inchi:	InChI=1S/C19H25Cl3O4/c1-2-11-25-17(23)9-7-5-3-4-6-8-10-18(24)26-14-12-15(20)19(22)
InchiKey:	GFZZFHVAQHAPNY-UHFFFAOYSA-N
Formula:	C19H25Cl3O4
SMILES:	CCCOC(=O)CCCCCCCCC(=O)Oc1cc(Cl)c(Cl)c(Cl)c1
Mol. weight [g/mol]:	423.76

Physical Properties

Property code	Value	Unit	Source
gf	-311.01	kJ/mol	Joback Method
hf	-770.19	kJ/mol	Joback Method
hfus	56.00	kJ/mol	Joback Method
hvap	93.62	kJ/mol	Joback Method
log10ws	-7.31		Crippen Method
logp	6.626		Crippen Method
mcvol	306.410	ml/mol	McGowan Method
pc	1298.60	kPa	Joback Method
rinqol	2961.00		NIST Webbook
tb	940.61	K	Joback Method
tc	1157.50	K	Joback Method
tf	601.95	K	Joback Method
vc	1.187	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	892.29	J/molxK	940.61	Joback Method
cpg	904.52	J/molxK	976.76	Joback Method
cpg	915.57	J/molxK	1012.91	Joback Method
cpg	925.46	J/molxK	1049.06	Joback Method
cpg	934.21	J/molxK	1085.21	Joback Method
cpg	941.84	J/molxK	1121.35	Joback Method
cpg	948.36	J/molxK	1157.50	Joback Method
dvisc	0.0002840	Paxs	601.95	Joback Method
dvisc	0.0001793	Paxs	658.39	Joback Method

dvisc	0.0001217	Paxs	714.84	Joback Method
dvisc	0.0000874	Paxs	771.28	Joback Method
dvisc	0.0000657	Paxs	827.72	Joback Method
dvisc	0.0000512	Paxs	884.17	Joback Method
dvisc	0.0000412	Paxs	940.61	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=U355220&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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