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

Inchi: InChI=1S/C19H25Cl3O4/c1-2-13-25-16(23)9-7-5-3-4-6-8-10-17(24)26-19-15(21)12-11-14
InchiKey: OHMHDLYXCZAMNL-UHFFFAOYSA-N
Formula: C19H25Cl3O4
SMILES: CCCOC(=O)CCCCCCCCC(=O)Oc1c(Cl)ccc(Cl)c1Cl
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
rinpol	2901.00		NIST Webbook
tb	940.61	K	Joback Method
tc	1157.50	K	Joback Method
tf	601.95	K	Joback Method
vc	1.187	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001217	Pa×s	714.84	Joback Method
dvisc	0.0000874	Pa×s	771.28	Joback Method
dvisc	0.0000657	Pa×s	827.72	Joback Method
dvisc	0.0000512	Pa×s	884.17	Joback Method
dvisc	0.0000412	Pa×s	940.61	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U355260&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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