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

Inchi: InChI=1S/C21H29Cl3O4/c1-2-3-10-15-27-18(25)11-8-6-4-5-7-9-12-19(26)28-21-17(23)14

InchiKey: XUNLIJKOPPMABH-UHFFFAOYSA-N

Formula: C21H29Cl3O4

SMILES: CCCCCOC(=O)CCCCCCCCC(=O)Oc1c(Cl)ccc(Cl)c1Cl

Mol. weight [g/mol]: 451.81

Physical Properties

Property code	Value	Unit	Source
gf	-294.17	kJ/mol	Joback Method
hf	-811.47	kJ/mol	Joback Method
hfus	61.18	kJ/mol	Joback Method
hvap	98.07	kJ/mol	Joback Method
log10ws	-8.14		Crippen Method
logp	7.406		Crippen Method
mcvol	334.590	ml/mol	McGowan Method
pc	1135.96	kPa	Joback Method
rinpol	3110.00		NIST Webbook
rinpol	3110.00		NIST Webbook
tb	986.37	K	Joback Method
tc	1208.66	K	Joback Method
tf	624.49	K	Joback Method
vc	1.298	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1010.15	J/mol×K	986.37	Joback Method
cpg	1022.76	J/mol×K	1023.42	Joback Method
cpg	1034.05	J/mol×K	1060.47	Joback Method
cpg	1044.06	J/mol×K	1097.52	Joback Method
cpg	1052.81	J/mol×K	1134.57	Joback Method
cpg	1060.33	J/mol×K	1171.62	Joback Method
cpg	1066.65	J/mol×K	1208.66	Joback Method
dvisc	0.0002266	Pa×s	624.49	Joback Method

dvisc	0.0001399	Pa×s	684.80	Joback Method
dvisc	0.0000934	Pa×s	745.12	Joback Method
dvisc	0.0000663	Pa×s	805.43	Joback Method
dvisc	0.0000493	Pa×s	865.74	Joback Method
dvisc	0.0000381	Pa×s	926.06	Joback Method
dvisc	0.0000304	Pa×s	986.37	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=U355263&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