

Sebacic acid, pentyl 2,4,5-trichlorophenyl ester

Inchi:	InChI=1S/C21H29Cl3O4/c1-2-3-10-13-27-20(25)11-8-6-4-5-7-9-12-21(26)28-19-15-17(2)
InchiKey:	OQOJORJWRIQQTP-UHFFFAOYSA-N
Formula:	C21H29Cl3O4
SMILES:	CCCCCOC(=O)CCCCCCCCC(=O)Oc1cc(Cl)c(Cl)cc1Cl
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
mvol	334.590	ml/mol	McGowan Method
pc	1135.96	kPa	Joback Method
rinpol	3111.00		NIST Webbook
rinpol	3111.00		NIST Webbook
tb	986.37	K	Joback Method
tc	1208.66	K	Joback Method
tf	624.49	K	Joback Method
vc	1.298	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001399	Paxs	684.80	Joback Method
dvisc	0.0000934	Paxs	745.12	Joback Method
dvisc	0.0000663	Paxs	805.43	Joback Method
dvisc	0.0000493	Paxs	865.74	Joback Method
dvisc	0.0000381	Paxs	926.06	Joback Method
dvisc	0.0000304	Paxs	986.37	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=U355194&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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