Glutaric acid, nonyl pentachlorophenyl ester

Inchi: InChI=1S/C20H25Cl5O4/c1-2-3-4-5-6-7-8-12-28-13(26)10-9-11-14(27)29-20-18(24)16(22
InchiKey: KYPOHHPNAMSWNW-UHFFFAOYSA-N
Formula: C20H25Cl5O4
SMILES: CCCCCCCCCOC(=O)CCCC(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 506.68

Physical Properties

Property code	Value	Unit	Source
gf	-345.71	kJ/mol	Joback Method
hf	-845.25	kJ/mol	Joback Method
hfus	66.21	kJ/mol	Joback Method
hvap	105.94	kJ/mol	Joback Method
log10ws	-9.10		Crippen Method
logp	8.323		Crippen Method
mcvol	344.980	ml/mol	McGowan Method
pc	1129.86	kPa	Joback Method
rinpol	3324.00		NIST Webbook
rinpol	3324.00		NIST Webbook
tb	1048.31	K	Joback Method
tc	1283.68	K	Joback Method
tf	698.10	K	Joback Method
vc	1.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	987.64	J/mol×K	1048.31	Joback Method
cpg	997.29	J/mol×K	1087.54	Joback Method
cpg	1005.53	J/mol×K	1126.77	Joback Method
cpg	1012.39	J/mol×K	1165.99	Joback Method
cpg	1017.88	J/mol×K	1205.22	Joback Method
cpg	1022.02	J/mol×K	1244.45	Joback Method
cpg	1024.82	J/mol×K	1283.68	Joback Method
dvisc	0.0001438	Pa×s	698.10	Joback Method

dvisc	0.0000970	Pa×s	756.47	Joback Method
dvisc	0.0000692	Pa×s	814.84	Joback Method
dvisc	0.0000517	Pa×s	873.20	Joback Method
dvisc	0.0000400	Pa×s	931.57	Joback Method
dvisc	0.0000319	Pa×s	989.94	Joback Method
dvisc	0.0000261	Pa×s	1048.31	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=U360259&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