Glutaric acid, pentachlorophenyl pentyl ester

Inchi: InChI=1S/C16H17Cl5O4/c1-2-3-4-8-24-9(22)6-5-7-10(23)25-16-14(20)12(18)11(17)13(19
InchiKey: SWCUXQIWCBQLNP-UHFFFAOYSA-N
Formula: C16H17Cl5O4
SMILES: CCCCCOC(=O)CCCC(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 450.57

Physical Properties

Property code	Value	Unit	Source
gf	-379.39	kJ/mol	Joback Method
hf	-762.69	kJ/mol	Joback Method
hfus	55.85	kJ/mol	Joback Method
hvap	97.03	kJ/mol	Joback Method
log10ws	-7.42		Crippen Method
logp	6.763		Crippen Method
mcvol	288.620	ml/mol	McGowan Method
pc	1489.58	kPa	Joback Method
rinpol	2904.00		NIST Webbook
rinpol	2904.00		NIST Webbook
tb	956.79	K	Joback Method
tc	1182.64	K	Joback Method
tf	653.02	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	757.16	J/mol×K	956.79	Joback Method
cpg	766.20	J/mol×K	994.43	Joback Method
cpg	774.14	J/mol×K	1032.07	Joback Method
cpg	780.96	J/mol×K	1069.72	Joback Method
cpg	786.66	J/mol×K	1107.36	Joback Method
cpg	791.26	J/mol×K	1145.00	Joback Method
cpg	794.73	J/mol×K	1182.64	Joback Method
dvisc	0.0002265	Pa×s	653.02	Joback Method

dvisc	0.0001594	Pa×s	703.65	Joback Method
dvisc	0.0001176	Pa×s	754.28	Joback Method
dvisc	0.0000902	Pa×s	804.90	Joback Method
dvisc	0.0000713	Pa×s	855.53	Joback Method
dvisc	0.0000579	Pa×s	906.16	Joback Method
dvisc	0.0000481	Pa×s	956.79	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=U360255&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