Glutaric acid, isobutyl pentachlorophenyl ester

Inchi: InChI=1S/C15H15Cl5O4/c1-7(2)6-23-8(21)4-3-5-9(22)24-15-13(19)11(17)10(16)12(18)14

InchiKey: RRRKJOCBHJXELM-UHFFFAOYSA-N

Formula: C15H15Cl5O4

SMILES: CC(C)COC(=O)CCCC(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl

Mol. weight [g/mol]: 436.54

Physical Properties

Property code	Value	Unit	Source
gf	-390.25	kJ/mol	Joback Method
hf	-747.33	kJ/mol	Joback Method
hfus	49.74	kJ/mol	Joback Method
hvap	94.42	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	6.228		Crippen Method
mcvol	274.530	ml/mol	McGowan Method
pc	1616.77	kPa	Joback Method
rinpol	2745.00		NIST Webbook
rinpol	2745.00		NIST Webbook
tb	933.47	K	Joback Method
tc	1161.44	K	Joback Method
tf	626.75	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	701.60	J/mol×K	933.47	Joback Method
cpg	734.95	J/mol×K	1123.44	Joback Method
cpg	730.48	J/mol×K	1085.45	Joback Method
cpg	724.90	J/mol×K	1047.45	Joback Method
cpg	718.23	J/mol×K	1009.46	Joback Method
cpg	710.46	J/mol×K	971.46	Joback Method
cpg	738.31	J/mol×K	1161.44	Joback Method
dvisc	0.0000509	Pa×s	933.47	Joback Method

dvisc	0.0000618	Pa×s	882.35	Joback Method
dvisc	0.0000769	Pa×s	831.23	Joback Method
dvisc	0.0000984	Pa×s	780.11	Joback Method
dvisc	0.0001304	Pa×s	728.99	Joback Method
dvisc	0.0001802	Pa×s	677.87	Joback Method
dvisc	0.0002627	Pa×s	626.75	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=U360253&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