Glutaric acid, isobutyl 2,3,5,6-tetrachlorophenyl ester

Inchi: InChI=1S/C15H16Cl4O4/c1-8(2)7-22-11(20)4-3-5-12(21)23-15-13(18)9(16)6-10(17)14(15

InchiKey: DCZJKKXXRFMGME-UHFFFAOYSA-N

Formula: C15H16Cl4O4

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

Mol. weight [g/mol]: 402.10

Physical Properties

Property code	Value	Unit	Source
gf	-368.69	kJ/mol	Joback Method
hf	-720.12	kJ/mol	Joback Method
hfus	45.93	kJ/mol	Joback Method
hvap	89.37	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	5.575		Crippen Method
mcvol	262.290	ml/mol	McGowan Method
pc	1686.56	kPa	Joback Method
rinpol	2587.00		NIST Webbook
rinpol	2587.00		NIST Webbook
tb	891.06	K	Joback Method
tc	1114.32	K	Joback Method
tf	584.31	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.41	J/mol×K	891.06	Joback Method
cpg	694.56	J/mol×K	928.27	Joback Method
cpg	703.66	J/mol×K	965.48	Joback Method
cpg	711.71	J/mol×K	1002.69	Joback Method
cpg	718.72	J/mol×K	1039.90	Joback Method
cpg	724.68	J/mol×K	1077.11	Joback Method
cpg	729.60	J/mol×K	1114.32	Joback Method
dvisc	0.0003459	Pa×s	584.31	Joback Method

dvisc	0.0002285	Pa×s	635.44	Joback Method
dvisc	0.0001606	Pa×s	686.56	Joback Method
dvisc	0.0001185	Pa×s	737.68	Joback Method
dvisc	0.0000909	Pa×s	788.81	Joback Method
dvisc	0.0000721	Pa×s	839.93	Joback Method
dvisc	0.0000587	Pa×s	891.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359317&Units=SI
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

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