

Glutaric acid, isobutyl 2,3,4,5-tetrachlorophenyl ester

Inchi: InChI=1S/C15H16Cl4O4/c1-8(2)7-22-11(20)4-3-5-12(21)23-10-6-9(16)13(17)15(19)14(10)2
InchiKey: VILJVEZXRLZXSL-UHFFFAOYSA-N
Formula: C15H16Cl4O4
SMILES: CC(C)COC(=O)CCCC(=O)Oc1cc(Cl)c(Cl)c(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	2615.00		NIST Webbook
rinpol	2615.00		NIST Webbook
tb	891.06	K	Joback Method
tc	1114.32	K	Joback Method
tf	584.31	K	Joback Method
vc	1.006	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0002285	Paxs	635.44	Joback Method
dvisc	0.0001606	Paxs	686.56	Joback Method
dvisc	0.0001185	Paxs	737.68	Joback Method
dvisc	0.0000909	Paxs	788.81	Joback Method
dvisc	0.0000721	Paxs	839.93	Joback Method
dvisc	0.0000587	Paxs	891.06	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U360748&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

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