Glutaric acid, 2,2-dichloroethyl pentafluorobenzyl ester

Inchi: InChI=1S/C14H11Cl2F5O4/c15-7(16)5-25-9(23)3-1-2-8(22)24-4-6-10(17)12(19)14(21)13

InchiKey: AOEKDQKAZJSCTC-UHFFFAOYSA-N

Formula: C14H11Cl2F5O4

SMILES: O=C(CCCC(=O)OCC(Cl)Cl)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 409.13

Physical Properties

Property code	Value	Unit	Source
gf	-1336.93	kJ/mol	Joback Method
hf	-1660.02	kJ/mol	Joback Method
hfus	49.96	kJ/mol	Joback Method
hvap	74.95	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	3.942		Crippen Method
mcvol	232.570	ml/mol	McGowan Method
pc	1593.62	kPa	Joback Method
rinpol	2064.00		NIST Webbook
rinpol	2064.00		NIST Webbook
tb	794.65	K	Joback Method
tc	984.86	K	Joback Method
tf	528.67	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.63	J/mol×K	794.65	Joback Method
cpg	633.64	J/mol×K	826.35	Joback Method
cpg	642.92	J/mol×K	858.05	Joback Method
cpg	651.46	J/mol×K	889.75	Joback Method
cpg	659.25	J/mol×K	921.46	Joback Method
cpg	666.30	J/mol×K	953.16	Joback Method
cpg	672.60	J/mol×K	984.86	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=U391931&Units=SI

Legend

cpg:	Ideal gas heat capacity
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