Glutaric acid, (2-chlorocyclohexyl)methyl 1,1,1-trifluoroprop-2-yl ester

Inchi: InChI=1S/C15H22ClF3O4/c1-10(15(17,18)19)23-14(21)8-4-7-13(20)22-9-11-5-2-3-6-12(1

InchiKey: FKBWOLRFPJODQT-UHFFFAOYSA-N

Formula: C15H22ClF3O4

SMILES: CC(OC(=O)CCCC(=O)OCC1CCCCC1Cl)C(F)(F)F

Mol. weight [g/mol]: 358.78

Physical Properties

Property code	Value	Unit	Source
gf	-971.64	kJ/mol	Joback Method
hf	-1426.65	kJ/mol	Joback Method
hfus	35.59	kJ/mol	Joback Method
hvap	67.67	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.992		Crippen Method
mcvol	243.780	ml/mol	McGowan Method
pc	1551.22	kPa	Joback Method
rinpol	1930.00		NIST Webbook
rinpol	1930.00		NIST Webbook
tb	741.63	K	Joback Method
tc	934.36	K	Joback Method
tf	425.38	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.13	J/mol×K	741.63	Joback Method
cpg	747.27	J/mol×K	773.75	Joback Method
cpg	762.33	J/mol×K	805.87	Joback Method
cpg	776.32	J/mol×K	837.99	Joback Method
cpg	789.27	J/mol×K	870.11	Joback Method
cpg	801.19	J/mol×K	902.24	Joback Method
cpg	812.12	J/mol×K	934.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405438&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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