Glutaric acid, 1,1,1-trifluoroprop-2-yl 4-chlorobenzyl ester

Inchi: InChI=1S/C15H16ClF3O4/c1-10(15(17,18)19)23-14(21)4-2-3-13(20)22-9-11-5-7-12(16)8

InchiKey: NNJXINGABOFNOQ-UHFFFAOYSA-N

Formula: C15H16ClF3O4

SMILES: CC(OC(=O)CCCC(=O)OCc1ccc(Cl)cc1)C(F)(F)F

Mol. weight [g/mol]: 352.73

Physical Properties

Property code	Value	Unit	Source
gf	-885.60	kJ/mol	Joback Method
hf	-1235.57	kJ/mol	Joback Method
hfus	36.33	kJ/mol	Joback Method
hvap	70.48	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.047		Crippen Method
mcvol	230.880	ml/mol	McGowan Method
pc	1743.37	kPa	Joback Method
rinpol	1951.00		NIST Webbook
rinpol	1951.00		NIST Webbook
tb	758.41	K	Joback Method
tc	956.61	K	Joback Method
tf	461.18	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	646.01	J/mol×K	758.41	Joback Method
cpg	658.57	J/mol×K	791.44	Joback Method
cpg	670.22	J/mol×K	824.48	Joback Method
cpg	681.00	J/mol×K	857.51	Joback Method
cpg	690.93	J/mol×K	890.54	Joback Method
cpg	700.04	J/mol×K	923.57	Joback Method
cpg	708.36	J/mol×K	956.61	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=U391720&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