Glutaric acid, (cyclohex-3-enyl)methyl 1,1,1-trifluoroprop-2-yl ester

Inchi: InChI=1S/C15H21F3O4/c1-11(15(16,17)18)22-14(20)9-5-8-13(19)21-10-12-6-3-2-4-7-12

InchiKey: SFSSQDJQFLXWMA-UHFFFAOYSA-N

Formula: C15H21F3O4

SMILES: CC(OC(=O)CCCC(=O)OCC1CC=CCC1)C(F)(F)F

Mol. weight [g/mol]: 322.32

Physical Properties

Property code	Value	Unit	Source
gf	-922.04	kJ/mol	Joback Method
hf	-1332.79	kJ/mol	Joback Method
hfus	31.54	kJ/mol	Joback Method
hvap	63.88	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.550		Crippen Method
mcvol	227.240	ml/mol	McGowan Method
pc	1689.34	kPa	Joback Method
rinpol	1737.00		NIST Webbook
rinpol	1737.00		NIST Webbook
tb	708.03	K	Joback Method
tc	897.93	K	Joback Method
tf	400.46	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	673.43	J/mol×K	708.03	Joback Method
cpg	689.49	J/mol×K	739.68	Joback Method
cpg	704.53	J/mol×K	771.33	Joback Method
cpg	718.57	J/mol×K	802.98	Joback Method
cpg	731.64	J/mol×K	834.63	Joback Method
cpg	743.77	J/mol×K	866.28	Joback Method
cpg	754.98	J/mol×K	897.93	Joback Method

Sources

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=U405520&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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