Glutaric acid, (cyclohex-3-enyl)methyl 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C15H20F4O4/c16-14(17)15(18,19)10-23-13(21)8-4-7-12(20)22-9-11-5-2-1-3-6

InchiKey: HWCBGHUGMQPIGP-UHFFFAOYSA-N

Formula: C15H20F4O4

SMILES: O=C(CCCC(=O)OCC(F)(F)C(F)F)OCC1CC=CCC1

Mol. weight [g/mol]: 340.31

Physical Properties

Property code	Value	Unit	Source
gf	-1116.85	kJ/mol	Joback Method
hf	-1528.90	kJ/mol	Joback Method
hfus	34.62	kJ/mol	Joback Method
hvap	63.07	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.500		Crippen Method
mcvol	229.010	ml/mol	McGowan Method
pc	1628.54	kPa	Joback Method
rinpol	1826.00		NIST Webbook
rinpol	1826.00		NIST Webbook
tb	707.30	K	Joback Method
tc	891.24	K	Joback Method
tf	401.05	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	681.25	J/mol×K	707.30	Joback Method
cpg	696.75	J/mol×K	737.96	Joback Method
cpg	711.28	J/mol×K	768.61	Joback Method
cpg	724.86	J/mol×K	799.27	Joback Method
cpg	737.53	J/mol×K	829.93	Joback Method
cpg	749.31	J/mol×K	860.59	Joback Method
cpg	760.22	J/mol×K	891.24	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=U405521&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