Glutaric acid, cyclohexylmethyl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C15H21F5O4/c16-14(17,15(18,19)20)10-24-13(22)8-4-7-12(21)23-9-11-5-2-1-
InchiKey: WKLSUJZIGJKSCL-UHFFFAOYSA-N
Formula: C15H21F5O4
SMILES: O=C(CCCC(=O)OCC(F)(F)C(F)(F)F)OCC1CCCCC1
Mol. weight [g/mol]: 360.32

Physical Properties

Property code	Value	Unit	Source
gf	-1336.34	kJ/mol	Joback Method
hf	-1786.26	kJ/mol	Joback Method
hfus	32.59	kJ/mol	Joback Method
hvap	61.05	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	4.021		Crippen Method
mcvol	235.080	ml/mol	McGowan Method
pc	1540.29	kPa	Joback Method
rinpol	1660.00		NIST Webbook
rinpol	1660.00		NIST Webbook
tb	704.62	K	Joback Method
tc	886.19	K	Joback Method
tf	418.30	K	Joback Method
vc	0.924	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	715.27	J/mol×K	704.62	Joback Method
cpg	731.20	J/mol×K	734.88	Joback Method
cpg	746.12	J/mol×K	765.14	Joback Method
cpg	760.07	J/mol×K	795.41	Joback Method
cpg	773.07	J/mol×K	825.67	Joback Method
cpg	785.18	J/mol×K	855.93	Joback Method
cpg	796.42	J/mol×K	886.19	Joback Method

Sources

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=U393674&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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