Glutaric acid, cyclohexylmethyl pentafluorobenzyl ester

Inchi: InChI=1S/C19H21F5O4/c20-15-12(16(21)18(23)19(24)17(15)22)10-28-14(26)8-4-7-13(25

InchiKey: VUJFOKJBJNVZGW-UHFFFAOYSA-N

Formula: C19H21F5O4

SMILES: O=C(CCCC(=O)OCC1CCCCC1)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 408.36

Physical Properties

Property code	Value	Unit	Source
gf	-1244.08	kJ/mol	Joback Method
hf	-1672.14	kJ/mol	Joback Method
hfus	49.87	kJ/mol	Joback Method
hvap	78.13	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	4.719		Crippen Method
mcvol	267.680	ml/mol	McGowan Method
pc	1357.63	kPa	Joback Method
rinpol	2293.00		NIST Webbook
rinpol	2293.00		NIST Webbook
tb	854.18	K	Joback Method
tc	1052.99	K	Joback Method
tf	547.56	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	847.65	J/mol×K	854.18	Joback Method
cpg	861.85	J/mol×K	887.31	Joback Method
cpg	874.87	J/mol×K	920.45	Joback Method
cpg	886.70	J/mol×K	953.58	Joback Method
cpg	897.35	J/mol×K	986.72	Joback Method
cpg	906.84	J/mol×K	1019.85	Joback Method
cpg	915.16	J/mol×K	1052.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391936&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

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