Glutaric acid, heptyl pentafluorobenzyl ester

Inchi: InChI=1S/C19H23F5O4/c1-2-3-4-5-6-10-27-13(25)8-7-9-14(26)28-11-12-15(20)17(22)19
InchiKey: YBOMQWLOEUIWEK-UHFFFAOYSA-N
Formula: C19H23F5O4
SMILES: CCCCCCCOC(=O)CCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 410.38

Physical Properties

Property code	Value	Unit	Source
gf	-1268.53	kJ/mol	Joback Method
hf	-1726.46	kJ/mol	Joback Method
hfus	58.04	kJ/mol	Joback Method
hvap	77.70	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	5.109		Crippen Method
mcvol	278.540	ml/mol	McGowan Method
pc	1173.63	kPa	Joback Method
rinpol	2272.00		NIST Webbook
tb	834.63	K	Joback Method
tc	1022.84	K	Joback Method
tf	540.18	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	853.27	J/mol×K	834.63	Joback Method
cpg	867.25	J/mol×K	866.00	Joback Method
cpg	880.27	J/mol×K	897.37	Joback Method
cpg	892.34	J/mol×K	928.73	Joback Method
cpg	903.45	J/mol×K	960.10	Joback Method
cpg	913.62	J/mol×K	991.47	Joback Method
cpg	922.84	J/mol×K	1022.84	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=U358872&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

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