Glutaric acid, hept-2-yl pentafluorobenzyl ester

Inchi: InChI=1S/C19H23F5O4/c1-3-4-5-7-11(2)28-14(26)9-6-8-13(25)27-10-12-15(20)17(22)19

InchiKey: LZFSPGCSTJFHAG-UHFFFAOYSA-N

Formula: C19H23F5O4

SMILES: CCCCCC(C)OC(=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	-1270.97	kJ/mol	Joback Method
hf	-1731.74	kJ/mol	Joback Method
hfus	54.51	kJ/mol	Joback Method
hvap	77.31	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	5.108		Crippen Method
mcvol	278.540	ml/mol	McGowan Method
pc	1180.09	kPa	Joback Method
rinpol	2089.00		NIST Webbook
rinpol	2089.00		NIST Webbook
tb	834.19	K	Joback Method
tc	1022.89	K	Joback Method
tf	525.18	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	853.81	J/mol×K	834.19	Joback Method
cpg	867.81	J/mol×K	865.64	Joback Method
cpg	880.85	J/mol×K	897.09	Joback Method
cpg	892.92	J/mol×K	928.54	Joback Method
cpg	904.02	J/mol×K	959.99	Joback Method
cpg	914.16	J/mol×K	991.44	Joback Method
cpg	923.35	J/mol×K	1022.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391933&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