Glutaric acid, dipentafluorobenzyl ester

Inchi: InChI=1S/C19H10F10O4/c20-10-6(11(21)15(25)18(28)14(10)24)4-32-8(30)2-1-3-9(31)33
InchiKey: QAUNIHZMXFZZBF-UHFFFAOYSA-N
Formula: C19H10F10O4
SMILES: O=C(CCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 492.26

Physical Properties

Property code	Value	Unit	Source
gf	-2178.32	kJ/mol	Joback Method
hf	-2527.83	kJ/mol	Joback Method
hfus	65.53	kJ/mol	Joback Method
hvap	79.20	kJ/mol	Joback Method
log10ws	-8.01		Crippen Method
logp	5.035		Crippen Method
mcvol	263.630	ml/mol	McGowan Method
pc	1198.96	kPa	Joback Method
rinpol	2234.00		NIST Webbook
rinpol	2234.00		NIST Webbook
tb	882.56	K	Joback Method
tc	1080.52	K	Joback Method
tf	632.15	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	786.26	J/mol×K	882.56	Joback Method
cpg	796.41	J/mol×K	915.55	Joback Method
cpg	805.57	J/mol×K	948.55	Joback Method
cpg	813.73	J/mol×K	981.54	Joback Method
cpg	820.86	J/mol×K	1014.54	Joback Method
cpg	826.97	J/mol×K	1047.53	Joback Method
cpg	832.03	J/mol×K	1080.52	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=U358884&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