Glutaric acid, isohexyl pentafluorobenzyl ester

Inchi: InChI=1S/C18H21F5O4/c1-10(2)5-4-8-26-12(24)6-3-7-13(25)27-9-11-14(19)16(21)18(23
InchiKey: GJDHJMHSYLSUDD-UHFFFAOYSA-N
Formula: C18H21F5O4
SMILES: CC(C)CCCOC(=O)CCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 396.35

Physical Properties

Property code	Value	Unit	Source
gf	-1279.39	kJ/mol	Joback Method
hf	-1711.10	kJ/mol	Joback Method
hfus	51.92	kJ/mol	Joback Method
hvap	75.09	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	4.575		Crippen Method
mcvol	264.450	ml/mol	McGowan Method
pc	1261.95	kPa	Joback Method
rinpol	2117.00		NIST Webbook
tb	811.31	K	Joback Method
tc	996.92	K	Joback Method
tf	513.91	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.29	J/mol×K	811.31	Joback Method
cpg	809.86	J/mol×K	842.25	Joback Method
cpg	822.54	J/mol×K	873.18	Joback Method
cpg	834.32	J/mol×K	904.12	Joback Method
cpg	845.21	J/mol×K	935.05	Joback Method
cpg	855.21	J/mol×K	965.99	Joback Method
cpg	864.31	J/mol×K	996.92	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=U358870&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