Glutaric acid, isobutyl pentafluorobenzyl ester

Inchi: InChI=1S/C16H17F5O4/c1-8(2)6-24-10(22)4-3-5-11(23)25-7-9-12(17)14(19)16(21)15(20
InchiKey: CJNAGPFAZANGLN-UHFFFAOYSA-N
Formula: C16H17F5O4
SMILES: CC(C)COC(=O)CCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 368.30

Physical Properties

Property code	Value	Unit	Source
gf	-1296.23	kJ/mol	Joback Method
hf	-1669.82	kJ/mol	Joback Method
hfus	46.74	kJ/mol	Joback Method
hvap	70.64	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	3.795		Crippen Method
mcvol	236.270	ml/mol	McGowan Method
pc	1453.46	kPa	Joback Method
rinpol	1915.00		NIST Webbook
rinpol	1915.00		NIST Webbook
tb	765.55	K	Joback Method
tc	947.17	K	Joback Method
tf	491.37	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.02	J/mol×K	765.55	Joback Method
cpg	696.68	J/mol×K	795.82	Joback Method
cpg	708.58	J/mol×K	826.09	Joback Method
cpg	719.71	J/mol×K	856.36	Joback Method
cpg	730.07	J/mol×K	886.63	Joback Method
cpg	739.66	J/mol×K	916.90	Joback Method
cpg	748.47	J/mol×K	947.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358867&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