Glutaric acid, butyl pentafluorobenzyl ester

Inchi: InChI=1S/C16H17F5O4/c1-2-3-7-24-10(22)5-4-6-11(23)25-8-9-12(17)14(19)16(21)15(20
InchiKey: SZBPFHILOTYCCK-UHFFFAOYSA-N
Formula: C16H17F5O4
SMILES: CCCCOC(=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	-1293.79	kJ/mol	Joback Method
hf	-1664.54	kJ/mol	Joback Method
hfus	50.27	kJ/mol	Joback Method
hvap	71.02	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	3.939		Crippen Method
mcvol	236.270	ml/mol	McGowan Method
pc	1444.64	kPa	Joback Method
rinpol	1963.00		NIST Webbook
rinpol	1963.00		NIST Webbook
tb	765.99	K	Joback Method
tc	946.20	K	Joback Method
tf	506.37	K	Joback Method
vc	0.962	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.46	J/mol×K	765.99	Joback Method
cpg	696.02	J/mol×K	796.02	Joback Method
cpg	707.82	J/mol×K	826.06	Joback Method
cpg	718.89	J/mol×K	856.09	Joback Method
cpg	729.20	J/mol×K	886.13	Joback Method
cpg	738.76	J/mol×K	916.16	Joback Method
cpg	747.57	J/mol×K	946.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358868&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