Glutaric acid, pentafluorobenzyl propyl ester

Inchi: InChI=1S/C15H15F5O4/c1-2-6-23-9(21)4-3-5-10(22)24-7-8-11(16)13(18)15(20)14(19)12
InchiKey: XEYOFORLHXVGAL-UHFFFAOYSA-N
Formula: C15H15F5O4
SMILES: CCCOC(=O)CCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 354.27

Physical Properties

Property code	Value	Unit	Source
gf	-1302.21	kJ/mol	Joback Method
hf	-1643.90	kJ/mol	Joback Method
hfus	47.68	kJ/mol	Joback Method
hvap	68.80	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	3.549		Crippen Method
mcvol	222.180	ml/mol	McGowan Method
pc	1556.12	kPa	Joback Method
rinpol	1866.00		NIST Webbook
rinpol	1866.00		NIST Webbook
tb	743.11	K	Joback Method
tc	922.01	K	Joback Method
tf	495.10	K	Joback Method
vc	0.905	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.88	J/mol×K	743.11	Joback Method
cpg	640.91	J/mol×K	772.93	Joback Method
cpg	652.27	J/mol×K	802.74	Joback Method
cpg	662.94	J/mol×K	832.56	Joback Method
cpg	672.92	J/mol×K	862.38	Joback Method
cpg	682.20	J/mol×K	892.19	Joback Method
cpg	690.77	J/mol×K	922.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358866&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