Pimelic acid, butyl pentafluorobenzyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-1276.95	kJ/mol	Joback Method
hf	-1705.82	kJ/mol	Joback Method
hfus	55.45	kJ/mol	Joback Method
hvap	75.47	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	4.719		Crippen Method
mcvol	264.450	ml/mol	McGowan Method
pc	1254.81	kPa	Joback Method
rinpol	2169.00		NIST Webbook
rinpol	2169.00		NIST Webbook
tb	811.75	K	Joback Method
tc	996.55	K	Joback Method
tf	528.91	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.74	J/mol×K	811.75	Joback Method
cpg	809.26	J/mol×K	842.55	Joback Method
cpg	821.89	J/mol×K	873.35	Joback Method
cpg	833.65	J/mol×K	904.15	Joback Method
cpg	844.53	J/mol×K	934.95	Joback Method
cpg	854.53	J/mol×K	965.75	Joback Method
cpg	863.66	J/mol×K	996.55	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=U416627&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