4-Piperidyl cyclopentylphenylglycolate

Inchi: InChI=1S/C18H25NO3/c20-17(22-16-10-12-19-13-11-16)18(21,15-8-4-5-9-15)14-6-2-1-3
InchiKey: MKFLPXGFTSXZKX-UHFFFAOYSA-N
Formula: C18H25NO3
SMILES: O=C(OC1CCNCC1)C(O)(c1ccccc1)C1CCCC1
Mol. weight [g/mol]: 303.40

Physical Properties

Property code	Value	Unit	Source
gf	-6.10	kJ/mol	Joback Method
hf	-431.49	kJ/mol	Joback Method
hfus	31.24	kJ/mol	Joback Method
hvap	89.92	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	2.360		Crippen Method
mcvol	242.290	ml/mol	McGowan Method
pc	2384.19	kPa	Joback Method
rinpol	2351.00		NIST Webbook
tb	886.54	K	Joback Method
tc	1127.25	K	Joback Method
tf	577.75	K	Joback Method
vc	0.878	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.85	J/mol×K	886.54	Joback Method
cpg	831.03	J/mol×K	926.66	Joback Method
cpg	845.66	J/mol×K	966.78	Joback Method
cpg	858.86	J/mol×K	1006.90	Joback Method
cpg	870.73	J/mol×K	1047.02	Joback Method
cpg	881.37	J/mol×K	1087.13	Joback Method
cpg	890.88	J/mol×K	1127.25	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=U289601&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