4-Piperidyl cyclohexylphenylglycolate

Inchi: InChI=1S/C19H27NO3/c21-18(23-17-11-13-20-14-12-17)19(22,15-7-3-1-4-8-15)16-9-5-2
InchiKey: SRYIVCXVRSNTJR-UHFFFAOYSA-N
Formula: C19H27NO3
SMILES: O=C(OC1CCNCC1)C(O)(c1ccccc1)C1CCCCC1
Mol. weight [g/mol]: 317.42

Physical Properties

Property code	Value	Unit	Source
gf	-9.78	kJ/mol	Joback Method
hf	-458.29	kJ/mol	Joback Method
hfus	31.73	kJ/mol	Joback Method
hvap	92.32	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	2.750		Crippen Method
mcvol	256.380	ml/mol	McGowan Method
pc	2227.09	kPa	Joback Method
rinpol	2445.00		NIST Webbook
rinpol	2445.00		NIST Webbook
tb	913.69	K	Joback Method
tc	1156.80	K	Joback Method
tf	585.50	K	Joback Method
vc	0.926	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.56	J/mol×K	913.69	Joback Method
cpg	893.77	J/mol×K	954.21	Joback Method
cpg	908.29	J/mol×K	994.73	Joback Method
cpg	921.22	J/mol×K	1035.24	Joback Method
cpg	932.65	J/mol×K	1075.76	Joback Method
cpg	942.68	J/mol×K	1116.28	Joback Method
cpg	951.41	J/mol×K	1156.80	Joback Method

Sources

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=U289602&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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