1-Methylcyclohexanyl anthranilate

Inchi: InChI=1S/C14H19NO2/c1-14(9-5-2-6-10-14)17-13(16)11-7-3-4-8-12(11)15/h3-4,7-8H,2,5
InchiKey: CLNJDWUPBRXNKC-UHFFFAOYSA-N
Formula: C14H19NO2
SMILES: CC1(OC(=O)c2ccccc2N)CCCCC1
Mol. weight [g/mol]: 233.31

Physical Properties

Property code	Value	Unit	Source
gf	21.27	kJ/mol	Joback Method
hf	-248.68	kJ/mol	Joback Method
hfus	19.19	kJ/mol	Joback Method
hvap	68.77	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.148		Crippen Method
mcvol	190.920	ml/mol	McGowan Method
pc	2790.61	kPa	Joback Method
rinpol	1922.70		NIST Webbook
rinpol	1922.70		NIST Webbook
tb	719.99	K	Joback Method
tc	970.47	K	Joback Method
tf	473.18	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.06	J/mol×K	719.99	Joback Method
cpg	566.23	J/mol×K	761.74	Joback Method
cpg	583.39	J/mol×K	803.48	Joback Method
cpg	599.71	J/mol×K	845.23	Joback Method
cpg	615.38	J/mol×K	886.98	Joback Method
cpg	630.57	J/mol×K	928.73	Joback Method
cpg	645.47	J/mol×K	970.47	Joback Method

Sources

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=U417238&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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