(+)-cis-2-Benzamidocyclohexane-carboxylic acid

Inchi: InChI=1S/C14H17NO3/c16-13(10-6-2-1-3-7-10)15-12-9-5-4-8-11(12)14(17)18/h1-3,6-7,1

InchiKey: PUANNVQABXUYKU-NEPJUHHUSA-N

Formula: C14H17NO3

SMILES: O=C(NC1CCCCC1C(=O)O)c1ccccc1

Mol. weight [g/mol]: 247.29

CAS: 26685-82-5

Physical Properties

Property code	Value	Unit	Source
gf	-109.12	kJ/mol	Joback Method
hf	-385.70	kJ/mol	Joback Method
hfus	31.35	kJ/mol	Joback Method
hvap	85.76	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	2.060		Crippen Method
mcvol	192.490	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
tb	811.37	K	Joback Method
tc	1035.91	K	Joback Method
tf	490.44	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.51	J/mol×K	811.37	Joback Method
cpg	605.86	J/mol×K	848.79	Joback Method
cpg	618.03	J/mol×K	886.22	Joback Method
cpg	629.09	J/mol×K	923.64	Joback Method
cpg	639.09	J/mol×K	961.06	Joback Method
cpg	648.07	J/mol×K	998.49	Joback Method
cpg	656.09	J/mol×K	1035.91	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=C26685825&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume