Benzoic acid, 2-amino-, cyclohexyl ester

Other names:	Anthranilic acid, cyclohexyl ester
	Cyclohexyl anthranilate
Inchi:	InChI=1S/C13H17NO2/c14-12-9-5-4-8-11(12)13(15)16-10-6-2-1-3-7-10/h4-5,8-10H,1-3,6
InchiKey:	KFEZETDKFSMLMG-UHFFFAOYSA-N
Formula:	C13H17NO2
SMILES:	Nc1ccccc1C(=O)OC1CCCCC1
Mol. weight [g/mol]:	219.28
CAS:	7779-16-0

Physical Properties

Property code	Value	Unit	Source
gf	18.34	kJ/mol	Joback Method
hf	-243.28	kJ/mol	Joback Method
hfus	22.90	kJ/mol	Joback Method
hvap	67.70	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	2.758		Crippen Method
mcvol	176.830	ml/mol	McGowan Method
pc	2947.28	kPa	Joback Method
tb	696.87	K	Joback Method
tc	943.61	K	Joback Method
tf	438.01	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.95	J/mol×K	696.87	Joback Method
cpg	516.53	J/mol×K	737.99	Joback Method
cpg	532.69	J/mol×K	779.12	Joback Method
cpg	547.47	J/mol×K	820.24	Joback Method
cpg	560.92	J/mol×K	861.36	Joback Method
cpg	573.08	J/mol×K	902.48	Joback Method
cpg	584.00	J/mol×K	943.61	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=C7779160&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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