

hexyl 4-aminobenzoate

Inchi:	InChI=1S/C13H19NO2/c1-2-3-4-5-10-16-13(15)11-6-8-12(14)9-7-11/h6-9H,2-5,10,14H2,
InchiKey:	UWIGKXXCHKVGHW-UHFFFAOYSA-N
Formula:	C13H19NO2
SMILES:	CCCCCCOC(=O)c1ccc(N)cc1
Mol. weight [g/mol]:	221.30
CAS:	13476-55-6

Physical Properties

Property code	Value	Unit	Source
gf	-6.11	kJ/mol	Joback Method
hf	-297.60	kJ/mol	Joback Method
hfus	31.06	kJ/mol	Joback Method
hvap	67.27	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.006		Crippen Method
mcvol	187.690	ml/mol	McGowan Method
pc	2386.52	kPa	Joback Method
tb	677.32	K	Joback Method
tc	888.49	K	Joback Method
tf	334.00 ± 1.00	K	NIST Webbook
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.18	J/molxK	677.32	Joback Method
cpg	522.08	J/molxK	712.51	Joback Method
cpg	536.07	J/molxK	747.71	Joback Method
cpg	549.17	J/molxK	782.90	Joback Method
cpg	561.42	J/molxK	818.10	Joback Method
cpg	572.83	J/molxK	853.29	Joback Method
cpg	583.43	J/molxK	888.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13476556&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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
mccvol:	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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