cis-3-Hexenyl anthranilate

Other names:	3-Hexen-1-ol, 2-aminobenzoate, (Z)-
	3-Hexen-ol, 2-aminobenzoate, (Z)-
	3-Hexen-1-yl 2-aminobenzoate
	cis-Hex-3-enyl anthranilate
	(3Z)-3-Hexenyl 2-aminobenzoate
	(Z)-3-Hexenyl anthranilate
	(Z)-Hex-3-enyl anthranilate
Inchi:	InChI=1S/C13H17NO2/c1-2-3-4-7-10-16-13(15)11-8-5-6-9-12(11)14/h3-6,8-9H,2,7,10,14
InchiKey:	VZWCCPAVZNSCEO-ARJAWSKDSA-N
Formula:	C13H17NO2
SMILES:	CCC=CCCOC(=O)c1ccccc1N
Mol. weight [g/mol]:	219.28
CAS:	65405-76-7

Physical Properties

Property code	Value	Unit	Source
gf	74.11	kJ/mol	Joback Method
hf	-180.38	kJ/mol	Joback Method
hfus	31.26	kJ/mol	Joback Method
hvap	67.23	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	2.782		Crippen Method
mcvol	183.390	ml/mol	McGowan Method
pc	2512.55	kPa	Joback Method
rinpol	1807.00		NIST Webbook
rinpol	1807.00		NIST Webbook
tb	681.48	K	Joback Method
tc	900.73	K	Joback Method
tf	425.55	K	Joback Method
vc	0.689	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	484.52	J/mol×K	681.48	Joback Method
cpg	498.85	J/mol×K	718.02	Joback Method
cpg	512.25	J/mol×K	754.56	Joback Method
cpg	524.77	J/mol×K	791.11	Joback Method
cpg	536.44	J/mol×K	827.65	Joback Method
cpg	547.31	J/mol×K	864.19	Joback Method
cpg	557.42	J/mol×K	900.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65405767&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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