

Citronellyl anthranilate

Other names:	6-Octen-1-ol, 3,7-dimethyl-, 2-aminobenzoate 3,7-dimethyloct-6-enyl 2-aminobenzoate
Inchi:	InChI=1S/C17H25NO2/c1-13(2)7-6-8-14(3)11-12-20-17(19)15-9-4-5-10-16(15)18/h4-5,7,
InchiKey:	LSJVMHIFWWGDY-UHFFFAOYSA-N
Formula:	C17H25NO2
SMILES:	CC(C)=CCCC(C)CCOC(=O)c1cccc1N
Mol. weight [g/mol]:	275.39
CAS:	68555-57-7

Physical Properties

Property code	Value	Unit	Source
gf	96.80	kJ/mol	Joback Method
hf	-278.01	kJ/mol	Joback Method
hfus	36.79	kJ/mol	Joback Method
hvap	75.82	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.198		Crippen Method
mvol	239.750	ml/mol	McGowan Method
pc	1786.37	kPa	Joback Method
rinpol	2201.40		NIST Webbook
rinpol	2201.40		NIST Webbook
tb	772.44	K	Joback Method
tc	986.16	K	Joback Method
tf	441.67	K	Joback Method
vc	0.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.93	J/molxK	772.44	Joback Method
cpg	717.18	J/molxK	808.06	Joback Method
cpg	732.39	J/molxK	843.68	Joback Method
cpg	746.59	J/molxK	879.30	Joback Method
cpg	759.85	J/molxK	914.92	Joback Method

cpg	772.21	J/mol×K	950.54	Joback Method
cpg	783.73	J/mol×K	986.16	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C68555577&Units=SI

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
hvp:	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

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