

Anthranilic acid, ester with vanillin

Inchi:	InChI=1S/C15H13NO4/c1-19-14-8-10(9-17)6-7-13(14)20-15(18)11-4-2-3-5-12(11)16/h2-5
InchiKey:	FYCZMGWISPAYSK-UHFFFAOYSA-N
Formula:	C15H13NO4
SMILES:	COc1cc(C=O)ccc1OC(=O)c1ccccc1N
Mol. weight [g/mol]:	271.27
CAS:	92553-90-7

Physical Properties

Property code	Value	Unit	Source
gf	-100.64	kJ/mol	Joback Method
hf	-343.09	kJ/mol	Joback Method
hfus	32.98	kJ/mol	Joback Method
hvap	84.45	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	2.309		Crippen Method
mcvol	199.550	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
rinpol	2492.30		NIST Webbook
rinpol	2492.30		NIST Webbook
tb	830.80	K	Joback Method
tc	1072.70	K	Joback Method
tf	568.86	K	Joback Method
vc	0.748	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.60	J/mol×K	830.80	Joback Method
cpg	571.04	J/mol×K	871.12	Joback Method
cpg	581.30	J/mol×K	911.43	Joback Method
cpg	590.40	J/mol×K	951.75	Joback Method
cpg	598.36	J/mol×K	992.07	Joback Method
cpg	605.18	J/mol×K	1032.38	Joback Method
cpg	610.89	J/mol×K	1072.70	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C92553907&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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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