

Linalyl anthranilate

Other names:	Anthranilic acid, 1,5-dimethyl-1-vinyl-4-hexenyl ester Linalyl anthranilate Anthranilic acid, linalyl ester 3,7-Dimethyl-1,6-octadien-3-yl, anthranilate 3,7-Dimethyl-1,6-octadien-3-yl o-aminobenzoate 1,5-Dimethyl-1-vinyl-4-hexen-1-yl o-aminobenzoate 4-Hexen-1-ol, 1,5-dimethyl-1-vinyl-, o-aminobenzoate Linalyl o-aminobenzoate 1,6-Octadien-3-ol, 3,7-dimethyl-, o-aminobenzoate 1,6-Octadien-3-ol, 3,7-dimethyl-, 3-(2-aminobenzoate) NSC 72026
Inchi:	InChI=1S/C17H23NO2/c1-5-17(4,12-8-9-13(2)3)20-16(19)14-10-6-7-11-15(14)18/h5-7,9-
InchiKey:	WHIJSULEEDNKPD-UHFFFAOYSA-N
Formula:	C17H23NO2
SMILES:	C=CC(C)(CCC=C(C)C)OC(=O)c1ccccc1N
Mol. weight [g/mol]:	273.38

Physical Properties

Property code	Value	Unit	Source
hfus	31.62	kJ/mol	Joback Method
logp	4.117		Crippen Method
mcvol	235.450	ml/mol	McGowan Method
rinpol	2057.00		NIST Webbook
rinpol	2057.00		NIST Webbook
rinpol	2157.00		NIST Webbook
rinpol	2157.00		NIST Webbook
tb	627.61	K	Cheméo Relay (1.0)
tf	292.83	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.76	J/mol×K	766.33	Joback Method
cpg	692.63	J/mol×K	803.58	Joback Method

cpg	707.42	J/mol×K	840.83	Joback Method
cpg	721.21	J/mol×K	878.08	Joback Method
cpg	734.08	J/mol×K	915.33	Joback Method
cpg	746.13	J/mol×K	952.58	Joback Method
cpg	757.43	J/mol×K	989.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7149260&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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