1,6-Octadien-3-ol, 3,7-dimethyl-, 2-aminobenzoate

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]: 273.37

CAS: 7149-26-0

Physical Properties

Property code	Value	Unit	Source
gf	189.92	kJ/mol	Joback Method
hf	-156.05	kJ/mol	Joback Method
hfus	31.62	kJ/mol	Joback Method
hvap	74.24	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.117		Crippen Method
mcvol	235.450	ml/mol	McGowan Method
pc	1869.17	kPa	Joback Method
rinpol	2157.00		NIST Webbook
rinpol	2057.00		NIST Webbook
rinpol	2057.00		NIST Webbook
rinpol	2157.00		NIST Webbook
tb	766.33	K	Joback Method
tc	989.83	K	Joback Method
tf	457.33	K	Joback Method
vc	0.883	m3/kmol	Joback Method

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
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