

O-nitro carbanilic acid, fenchyl ester

Inchi:	InChI=1S/C17H22N2O4/c1-16(2)11-8-9-17(3,10-11)14(16)23-15(20)18-12-6-4-5-7-13(12)
InchiKey:	OIYUUVKTZUFWQH-UHFFFAOYSA-N
Formula:	C17H22N2O4
SMILES:	CC12CCC(C1)C(C)(C)C2OC(=O)Nc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	318.37
CAS:	93437-08-2

Physical Properties

Property code	Value	Unit	Source
gf	169.06	kJ/mol	Joback Method
hf	-242.00	kJ/mol	Joback Method
hfus	36.40	kJ/mol	Joback Method
hvap	85.63	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.358		Crippen Method
mcvol	239.750	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
tb	907.21	K	Joback Method
tc	1160.91	K	Joback Method
tf	660.40	K	Joback Method
vc	0.920	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	804.86	J/molxK	907.21	Joback Method
cpg	827.00	J/molxK	949.49	Joback Method
cpg	850.06	J/molxK	991.78	Joback Method
cpg	874.43	J/molxK	1034.06	Joback Method
cpg	900.50	J/molxK	1076.35	Joback Method
cpg	928.68	J/molxK	1118.63	Joback Method
cpg	959.34	J/molxK	1160.91	Joback Method

Sources

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=C93437082&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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