

Butralin

Other names:	Benzenamine, 4-(1,1-dimethylethyl)-N-(1-methylpropyl)-2,6-dinitro- Aniline, N-sec-butyl-4-tert-butyl-2,6-dinitro- A 820 Amchem 70-25 Amex Amex 820 Butalin Dibutalin N-sec-Butyl-4-tert-butyl-2,6-dinitroaniline 70-314B 72-A34 Amchem A-280 Butraline 4-(1,1-Dimethylethyl)-N-(1-methylpropyl)-2,6-dinitrobenzenamine Rutralin Tamex 4-(tert-Butyl)-N-sec-butyl-2,6-dinitroaniline 4-(1,1-Dimethylethyl)-N-(1-methylpropyl)-2,6-dinitrobenzeneamine
Inchi:	InChI=1S/C14H21N3O4/c1-6-9(2)15-13-11(16(18)19)7-10(14(3,4)5)8-12(13)17(20)21/h7
InchiKey:	SPNQRCTZKIBOAX-UHFFFAOYSA-N
Formula:	C14H21N3O4
SMILES:	CCC(C)Nc1c([N+](=O)[O-])cc(C(C)(C)C)cc1[N+](=O)[O-]
Mol. weight [g/mol]:	295.33
CAS:	33629-47-9

Physical Properties

Property code	Value	Unit	Source
gf	311.41	kJ/mol	Joback Method
hf	-112.25	kJ/mol	Joback Method
hfus	41.77	kJ/mol	Joback Method
hvap	88.95	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	4.011		Crippen Method
mcvol	229.180	ml/mol	McGowan Method
pc	2043.76	kPa	Joback Method
tb	911.52	K	Joback Method
tc	1161.78	K	Joback Method

tf	332.47 ± 0.20	K	NIST Webbook
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.22	J/molxK	911.52	Joback Method
cpg	732.10	J/molxK	953.23	Joback Method
cpg	743.94	J/molxK	994.94	Joback Method
cpg	754.85	J/molxK	1036.65	Joback Method
cpg	764.92	J/molxK	1078.36	Joback Method
cpg	774.26	J/molxK	1120.07	Joback Method
cpg	782.96	J/molxK	1161.78	Joback Method
hfust	20.84	kJ/mol	338.80	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33629479&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

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
hfust:	Enthalpy of fusion at a given temperature
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

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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