Benzenesulfonamide, 3-amino-N-butyl-4-methoxy-

Other names: Azoene Fast Red PDC Base
C.I. Azoic Diazo Component 14
C.I. 37151
Fast Ponceau L Base
Fast Red Base SW
Fast Red Ponceau L base
Fast Red PDC Base
Fast Red SW Base
Fast Red SW Special Base
Hiltonil Fast Red PDC Base
Metanilamide, N1-butyl-4-methoxy-
N'-Butyl-4-methoxymetanilamide
N1-Butyl-4-methoxymetanilamide
Red PDC Base
N'-n-Butyl-3-amino-4-methoxybenzenesulfonamide
NSC 50673
3-amino-N-butyl-4-methoxybenzenesulphonamide

Inchi: InChI=1S/C11H18N2O3S/c1-3-4-7-13-17(14,15)9-5-6-11(16-2)10(12)8-9/h5-6,8,13H,3-4

InchiKey: XOIMPHNXVTYJAB-UHFFFAOYSA-N

Formula: C11H18N2O3S

SMILES: CCCCNS(=O)(=O)c1ccc(OC)c(N)c1

Mol. weight [g/mol]: 258.34

CAS: 80-22-8

Physical Properties

Property code	Value	Unit	Source
gf	-282.81	kJ/mol	Joback Method
hf	-555.09	kJ/mol	Joback Method
hfus	40.37	kJ/mol	Joback Method
hvap	81.80	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	1.356		Crippen Method
mcvol	196.010	ml/mol	McGowan Method
pc	3210.04	kPa	Joback Method
tb	680.62	K	Joback Method
tc	885.25	K	Joback Method
tf	461.90	K	Joback Method

vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.93	J/mol×K	680.62	Joback Method
cpg	539.18	J/mol×K	714.72	Joback Method
cpg	552.51	J/mol×K	748.83	Joback Method
cpg	564.95	J/mol×K	782.93	Joback Method
cpg	576.47	J/mol×K	817.04	Joback Method
cpg	587.09	J/mol×K	851.14	Joback Method
cpg	596.80	J/mol×K	885.25	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C80228&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
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