Captodiamine

Other names: Ethanamine, 2-[[[4-(butylthio)phenyl]phenylmethyl]thio]-N,N-dimethyl-
Ethylamine, 2-[[p-(butylthio)-«alpha»-phenylbenzyl]thio]-N,N-dimethyl-
p-Butylmercaptobenzhydryl «beta»-dimethylaminoethyl sulfide
p-Butylthiodiphenylmethyl 2-(dimethylamino)ethyl sulfide
Captodiam
Captodiame
Captodiamin
Captodramin
Captodramine
Covatin
Covatix
p-Butylmercaptobenzhydryl-«beta»-dimethylamino-ethylsulphide
2-((p-(Butylthio)-«alpha»-phenylbenzyl)thio)-N,N-dimethylethylamine
Kaptodiamin
N 68
VUFB 2350

Inchi: InChI=1S/C21H29NS2/c1-4-5-16-23-20-13-11-19(12-14-20)21(24-17-15-22(2)3)18-9-7-6

InchiKey: IZLPZXSZLLELBJ-UHFFFAOYSA-N

Formula: C21H29NS2

SMILES: CCCCSc1ccc(C(SCCN(C)C)c2ccccc2)cc1

Mol. weight [g/mol]: 359.59

CAS: 486-17-9

Physical Properties

Property code	Value	Unit	Source
gf	515.71	kJ/mol	Joback Method
hf	130.81	kJ/mol	Joback Method
hfus	45.60	kJ/mol	Joback Method
hvap	82.84	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.963		Crippen Method
mcvol	301.910	ml/mol	McGowan Method
pc	1541.49	kPa	Joback Method
rinpol	2774.00		NIST Webbook
tb	887.78	K	Joback Method
tc	1127.69	K	Joback Method
tf	478.06	K	Joback Method

vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	910.63	J/mol×K	887.78	Joback Method
cpg	927.54	J/mol×K	927.76	Joback Method
cpg	942.97	J/mol×K	967.75	Joback Method
cpg	957.01	J/mol×K	1007.73	Joback Method
cpg	969.76	J/mol×K	1047.72	Joback Method
cpg	981.31	J/mol×K	1087.70	Joback Method
cpg	991.76	J/mol×K	1127.69	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C486179&Units=SI

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