

Cyheptamide

Other names:

5H-Dibenzo[a,d]cycloheptene-5-carboxamide, 10,11-dihydro-
AY 8682
BS 7029
Cyheptamine
Dibenzo(a,d)cycloheptadiene-5-carboxamide
Dibenzo(a,d)(1,4)-cycloheptadiene-5-carboxamide
10,11-Dihydro-5H-dibenzo(a,d)cycloheptene-5-carboxamide
ICI 51426
Carbamazepam
Cyhetamide

Inchi:

InChI=1S/C16H15NO/c17-16(18)15-13-7-3-1-5-11(13)9-10-12-6-2-4-8-14(12)15/h1-8,15

InchiKey:

APBVLLORZMAWKI-UHFFFAOYSA-N

Formula:

C16H15NO

SMILES:

NC(=O)C1c2ccccc2CCc2ccccc21

Mol. weight [g/mol]:

237.30

CAS:

7199-29-3

Physical Properties

Property code	Value	Unit	Source
gf	287.68	kJ/mol	Joback Method
hf	70.56	kJ/mol	Joback Method
hfus	29.43	kJ/mol	Joback Method
hvap	74.39	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	2.402		Crippen Method
mcvol	189.470	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
rinpol	2266.00		NIST Webbook
rinpol	2358.80		NIST Webbook
rinpol	2358.80		NIST Webbook
tb	761.94	K	Joback Method
tc	1020.72	K	Joback Method
tf	499.09	K	Joback Method
vc	0.708	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.22	J/mol×K	761.94	Joback Method
cpg	551.42	J/mol×K	805.07	Joback Method
cpg	565.37	J/mol×K	848.20	Joback Method
cpg	578.18	J/mol×K	891.33	Joback Method
cpg	590.01	J/mol×K	934.46	Joback Method
cpg	600.97	J/mol×K	977.59	Joback Method
cpg	611.22	J/mol×K	1020.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7199293&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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