Benzothiopyran, 4h-1-, 4-(3-(2-chloroethyl)ureido)-2,3-dl-hydro-

Inchi: InChI=1S/C12H15ClN2OS/c13-6-7-14-12(16)15-10-5-8-17-11-4-2-1-3-9(10)11/h1-4,10H,

InchiKey: FPMGZVWNTSTEOW-UHFFFAOYSA-N

Formula: C12H15ClN2OS

SMILES: O=C(NCCCl)NC1CCSc2ccccc21

Mol. weight [g/mol]: 270.78

CAS: 27047-62-7

Physical Properties

Property code	Value	Unit	Source
gf	279.38	kJ/mol	Joback Method
hf	24.57	kJ/mol	Joback Method
hfus	36.17	kJ/mol	Joback Method
hvap	75.14	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	2.762		Crippen Method
mcvol	195.440	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
tb	756.10	K	Joback Method
tc	996.98	K	Joback Method
tf	546.98	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.09	J/mol×K	756.10	Joback Method
cpg	541.64	J/mol×K	796.25	Joback Method
cpg	554.11	J/mol×K	836.39	Joback Method
cpg	565.61	J/mol×K	876.54	Joback Method
cpg	576.22	J/mol×K	916.69	Joback Method
cpg	586.02	J/mol×K	956.84	Joback Method
cpg	595.11	J/mol×K	996.98	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=C27047627&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume