Benzoic acid, m-[3-(2-chloroethyl)ureido]-

Inchi: InChI=1S/C10H11ClN2O3/c11-4-5-12-10(16)13-8-3-1-2-7(6-8)9(14)15/h1-3,6H,4-5H2,(H
InchiKey: SSRMHTGBJOCURP-UHFFFAOYSA-N
Formula: C10H11ClN2O3
SMILES: O=C(NCCCl)Nc1cccc(C(=O)O)c1
Mol. weight [g/mol]: 242.66
CAS: 13908-45-7

Physical Properties

Property code	Value	Unit	Source
gf	-91.71	kJ/mol	Joback Method
hf	-310.86	kJ/mol	Joback Method
hfus	36.99	kJ/mol	Joback Method
hvap	88.22	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	1.745		Crippen Method
mcvol	169.210	ml/mol	McGowan Method
pc	3650.93	kPa	Joback Method
tb	797.55	K	Joback Method
tc	1009.55	K	Joback Method
tf	537.32	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.98	J/mol×K	797.55	Joback Method
cpg	460.53	J/mol×K	832.88	Joback Method
cpg	468.41	J/mol×K	868.22	Joback Method
cpg	475.65	J/mol×K	903.55	Joback Method
cpg	482.28	J/mol×K	938.88	Joback Method
cpg	488.35	J/mol×K	974.21	Joback Method
cpg	493.87	J/mol×K	1009.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13908457&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