

Glutaramic acid, 2-[3-(2-chloroethyl)ureido]-, I(-)

Inchi:	InChI=1S/C8H14ClN3O4/c9-3-4-11-8(16)12-5(7(14)15)1-2-6(10)13/h5H,1-4H2,(H2,10,13)
InchiKey:	BJNJLMYPSUMCTL-UHFFFAOYSA-N
Formula:	C8H14ClN3O4
SMILES:	NC(=O)CCC(NC(=O)NCCCl)C(=O)O
Mol. weight [g/mol]:	251.67
CAS:	13908-05-9

Physical Properties

Property code	Value	Unit	Source
gf	-276.24	kJ/mol	Joback Method
hf	-578.71	kJ/mol	Joback Method
hfus	41.43	kJ/mol	Joback Method
hvap	97.83	kJ/mol	Joback Method
log10ws	-0.88		Crippen Method
logp	-0.757		Crippen Method
mcvol	176.340	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
tb	846.09	K	Joback Method
tc	1051.03	K	Joback Method
tf	594.03	K	Joback Method
vc	0.662	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.53	J/molxK	846.09	Joback Method
cpg	513.42	J/molxK	880.25	Joback Method
cpg	520.69	J/molxK	914.40	Joback Method
cpg	527.36	J/molxK	948.56	Joback Method
cpg	533.47	J/molxK	982.71	Joback Method
cpg	539.02	J/molxK	1016.87	Joback Method
cpg	544.06	J/molxK	1051.03	Joback Method

Sources

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=C13908059&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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