SIGMODAL

Inchi: InChI=1S/C12H17BrN2O3/c1-4-5-7(2)12(6-8(3)13)9(16)14-11(18)15-10(12)17/h7H,3-6H
InchiKey: ZGVCLZRQOUEZHG-UHFFFAOYSA-N
Formula: C12H17BrN2O3
SMILES: C=C(Br)CC1(C(C)CCC)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]: 317.18

Physical Properties

Property code	Value	Unit	Source
hfus	29.26	kJ/mol	Joback Method
log10ws	-3.40		Cheméo Relay (1.0)
logp	2.074		Crippen Method
mcvol	206.950	ml/mol	McGowan Method
tf	411.72	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.74	J/mol×K	856.59	Joback Method
cpg	636.04	J/mol×K	900.66	Joback Method
cpg	652.35	J/mol×K	944.72	Joback Method
cpg	667.72	J/mol×K	988.79	Joback Method
cpg	682.19	J/mol×K	1032.86	Joback Method
cpg	695.82	J/mol×K	1076.92	Joback Method
cpg	708.64	J/mol×K	1120.99	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1216406&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point