Iodamide

Inchi: InChI=1S/C12H11I3N2O4/c1-4(18)16-3-6-8(13)7(12(20)21)10(15)11(9(6)14)17-5(2)19/h3
InchiKey: VVDGWALACJEJKG-UHFFFAOYSA-N
Formula: C12H11I3N2O4
SMILES: CC(=O)NCc1c(I)c(NC(C)=O)c(I)c(C(=O)O)c1I
Mol. weight [g/mol]: 627.94
CAS: 440-58-4

Physical Properties

Property code	Value	Unit	Source
hfus	55.69	kJ/mol	Joback Method
log10ws	-3.47		Cheméo Relay (1.0)
logp	2.793		Crippen Method
mcvol	264.180	ml/mol	McGowan Method
tf	528.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	8.15410e+01
Coeff. B	1.03164e+00
Coeff. C	-7.01600e-04
Coeff. D	1.83220e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637
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

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

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