7-Aminonitrazepam

Inchi: InChI=1S/C15H13N3O/c16-11-6-7-13-12(8-11)15(17-9-14(19)18-13)10-4-2-1-3-5-10/h1-8
InchiKey: OYOUQHVDCKOOAL-UHFFFAOYSA-N
Formula: C15H13N3O
SMILES: Nc1ccc2c(c1)C(c1ccccc1)=NCC(=O)N2
Mol. weight [g/mol]: 251.29

Physical Properties

Property code	Value	Unit	Source
hfus	35.04	kJ/mol	Joback Method
log10ws	-2.71		Cheméo Relay (1.0)
logp	2.058		Crippen Method
mcvol	191.040	ml/mol	McGowan Method
tf	517.88	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.75	J/mol×K	872.61	Joback Method
cpg	595.51	J/mol×K	921.46	Joback Method
cpg	607.21	J/mol×K	970.30	Joback Method
cpg	616.86	J/mol×K	1019.15	Joback Method
cpg	624.46	J/mol×K	1067.99	Joback Method
cpg	630.05	J/mol×K	1116.84	Joback Method
cpg	633.62	J/mol×K	1165.69	Joback Method

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4928023&Units=SI
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):	

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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