

1-Adamantanecarboxamide, N-tetrahydrofurfuryl-

Inchi: InChI=1S/C16H25NO2/c18-15(17-10-14-2-1-3-19-14)16-7-11-4-12(8-16)6-13(5-11)9-16/
InchiKey: ZTLHMUKWSKSSEP-UHFFFAOYSA-N
Formula: C16H25NO2
SMILES: O=C(NCC1CCCO1)C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 263.38

Physical Properties

Property code	Value	Unit	Source
gf	151.69	kJ/mol	Joback Method
hf	-297.06	kJ/mol	Joback Method
hfus	32.89	kJ/mol	Joback Method
hvap	67.61	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.498		Crippen Method
mcvol	210.280	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
rinpol	2210.00		NIST Webbook
rinpol	2210.00		NIST Webbook
tb	731.81	K	Joback Method
tc	965.94	K	Joback Method
tf	480.10	K	Joback Method
vc	0.794	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.47	J/mol×K	731.81	Joback Method
cpg	714.96	J/mol×K	770.83	Joback Method
cpg	735.39	J/mol×K	809.85	Joback Method
cpg	755.02	J/mol×K	848.88	Joback Method
cpg	774.13	J/mol×K	887.90	Joback Method
cpg	792.97	J/mol×K	926.92	Joback Method
cpg	811.82	J/mol×K	965.94	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=U307464&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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