

Benzamide, 4-methyl-N-(hept-2-yl)-

Inchi:	InChI=1S/C15H23NO/c1-4-5-6-7-13(3)16-15(17)14-10-8-12(2)9-11-14/h8-11,13H,4-7H2,
InchiKey:	ZKRXZMYQHZOKFU-UHFFFAOYSA-N
Formula:	C15H23NO
SMILES:	CCCCC(C)NC(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	233.35

Physical Properties

Property code	Value	Unit	Source
gf	136.23	kJ/mol	Joback Method
hf	-192.26	kJ/mol	Joback Method
hfus	31.43	kJ/mol	Joback Method
hvap	64.72	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	3.694		Crippen Method
mcvol	210.000	ml/mol	McGowan Method
pc	1961.34	kPa	Joback Method
rinqol	1969.00		NIST Webbook
tb	677.86	K	Joback Method
tc	881.81	K	Joback Method
tf	385.34	K	Joback Method
vc	0.802	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.38	J/molxK	677.86	Joback Method
cpg	592.11	J/molxK	711.85	Joback Method
cpg	607.84	J/molxK	745.84	Joback Method
cpg	622.63	J/molxK	779.84	Joback Method
cpg	636.50	J/molxK	813.83	Joback Method
cpg	649.50	J/molxK	847.82	Joback Method
cpg	661.67	J/molxK	881.81	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=U407469&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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