

Benzamide, 4-ethyl-N-butyl-N-hept-2-yl-

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C20H33NO/c1-5-8-10-11-17(4)21(16-9-6-2)20(22)19-14-12-18(7-3)13-15-19/h

JARFLYQQSIEPGV-UHFFFAOYSA-N

C20H33NO

CCCCC(C)N(CCCC)C(=O)c1ccc(CC)cc1

303.48

Physical Properties

Property code	Value	Unit	Source
gf	199.72	kJ/mol	Joback Method
hf	-281.40	kJ/mol	Joback Method
hfus	42.30	kJ/mol	Joback Method
hvap	71.45	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	5.460		Crippen Method
mcvol	280.450	ml/mol	McGowan Method
pc	1319.43	kPa	Joback Method
rinpol	2739.00		NIST Webbook
rinpol	2739.00		NIST Webbook
tb	754.53	K	Joback Method
tc	947.21	K	Joback Method
tf	421.50	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	837.92	J/mol×K	754.53	Joback Method
cpg	856.78	J/mol×K	786.64	Joback Method
cpg	874.57	J/mol×K	818.76	Joback Method
cpg	891.33	J/mol×K	850.87	Joback Method
cpg	907.12	J/mol×K	882.98	Joback Method
cpg	921.97	J/mol×K	915.09	Joback Method
cpg	935.95	J/mol×K	947.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415892&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hvap:	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
rinsol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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