

Acetamide, 2-phenyl-N-butyl-N-2-ethylhexyl-

Inchi:	InChI=1S/C20H33NO/c1-4-7-12-18(6-3)17-21(15-8-5-2)20(22)16-19-13-10-9-11-14-19/h
InchiKey:	CQQQBMJDTJLIJK-UHFFFAOYSA-N
Formula:	C20H33NO
SMILES:	CCCCC(CC)CN(CCCC)C(=O)Cc1ccccc1
Mol. weight [g/mol]:	303.48

Physical Properties

Property code	Value	Unit	Source
gf	209.35	kJ/mol	Joback Method
hf	-269.93	kJ/mol	Joback Method
hfus	42.69	kJ/mol	Joback Method
hvap	70.79	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	5.074		Crippen Method
mcvol	280.450	ml/mol	McGowan Method
pc	1333.93	kPa	Joback Method
rinpol	1641.00		NIST Webbook
tb	749.55	K	Joback Method
tc	941.39	K	Joback Method
tf	408.98	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	838.00	J/mol×K	749.55	Joback Method
cpg	856.97	J/mol×K	781.52	Joback Method
cpg	874.86	J/mol×K	813.50	Joback Method
cpg	891.70	J/mol×K	845.47	Joback Method
cpg	907.56	J/mol×K	877.45	Joback Method
cpg	922.49	J/mol×K	909.42	Joback Method
cpg	936.54	J/mol×K	941.39	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415675&Units=SI

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
mcvol:	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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