Benzamide, 4-butyl-N-(2-ethylhexyl)-

Inchi: InChI=1S/C19H31NO/c1-4-7-9-16(6-3)15-20-19(21)18-13-11-17(12-14-18)10-8-5-2/h11-1
InchiKey: IAVZWWHYHSTCCU-UHFFFAOYSA-N
Formula: C19H31NO
SMILES: CCCCc1ccc(C(=O)NCC(CC)CCCC)cc1
Mol. weight [g/mol]: 289.46

Physical Properties

Property code	Value	Unit	Source
gf	169.91	kJ/mol	Joback Method
hf	-274.82	kJ/mol	Joback Method
hfus	41.79	kJ/mol	Joback Method
hvap	73.62	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	4.975		Crippen Method
mcvol	266.360	ml/mol	McGowan Method
pc	1432.63	kPa	Joback Method
rinpol	2406.00		NIST Webbook
rinpol	2406.00		NIST Webbook
tb	769.38	K	Joback Method
tc	966.37	K	Joback Method
tf	430.42	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	799.78	J/mol×K	769.38	Joback Method
cpg	817.60	J/mol×K	802.21	Joback Method
cpg	834.38	J/mol×K	835.04	Joback Method
cpg	850.15	J/mol×K	867.87	Joback Method
cpg	864.97	J/mol×K	900.71	Joback Method
cpg	878.88	J/mol×K	933.54	Joback Method
cpg	891.92	J/mol×K	966.37	Joback Method

Sources

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=U407453&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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