

Butanamide, N,N-dioctyl-

Inchi:	InChI=1S/C20H41NO/c1-4-7-9-11-13-15-18-21(20(22)17-6-3)19-16-14-12-10-8-5-2/h4-1
InchiKey:	YTHTWWXHLQCJRN-UHFFFAOYSA-N
Formula:	C20H41NO
SMILES:	CCCCCCCCN(CCCCCCCC)C(=O)CCC
Mol. weight [g/mol]:	311.55

Physical Properties

Property code	Value	Unit	Source
gf	99.38	kJ/mol	Joback Method
hf	-501.18	kJ/mol	Joback Method
hfus	52.18	kJ/mol	Joback Method
hvap	68.90	kJ/mol	Joback Method
log10ws	-6.54		Crippen Method
logp	6.336		Crippen Method
mcvol	304.210	ml/mol	McGowan Method
pc	1056.20	kPa	Joback Method
rinsol	2168.00		NIST Webbook
tb	723.31	K	Joback Method
tc	893.05	K	Joback Method
tf	397.56	K	Joback Method
vc	1.179	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	918.49	J/mol×K	723.31	Joback Method
cpg	938.52	J/mol×K	751.60	Joback Method
cpg	957.61	J/mol×K	779.89	Joback Method
cpg	975.81	J/mol×K	808.18	Joback Method
cpg	993.15	J/mol×K	836.47	Joback Method
cpg	1009.65	J/mol×K	864.76	Joback Method
cpg	1025.37	J/mol×K	893.05	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=U308681&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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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