Pentanamide, N,N-dibutyl-

Inchi: InChI=1S/C13H27NO/c1-4-7-10-13(15)14(11-8-5-2)12-9-6-3/h4-12H2,1-3H3
InchiKey: VXZDQWAMPQZQQL-UHFFFAOYSA-N
Formula: C13H27NO
SMILES: CCCCC(=O)N(CCCC)CCCC
Mol. weight [g/mol]: 213.36

Physical Properties

Property code	Value	Unit	Source
gf	40.44	kJ/mol	Joback Method
hf	-356.70	kJ/mol	Joback Method
hfus	34.05	kJ/mol	Joback Method
hvap	53.32	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	3.605		Crippen Method
mcvol	205.580	ml/mol	McGowan Method
pc	1728.90	kPa	Joback Method
rinpol	1555.00		NIST Webbook
rinpol	1555.00		NIST Webbook
tb	563.15	K	Joback Method
tc	730.89	K	Joback Method
tf	318.67	K	Joback Method
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.59	J/mol×K	563.15	Joback Method
cpg	540.63	J/mol×K	591.11	Joback Method
cpg	556.92	J/mol×K	619.06	Joback Method
cpg	572.50	J/mol×K	647.02	Joback Method
cpg	587.39	J/mol×K	674.98	Joback Method
cpg	601.60	J/mol×K	702.94	Joback Method
cpg	615.17	J/mol×K	730.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308178&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
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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