Pentanamide, N,N-dioctyl-5-bromo-

Inchi: InChI=1S/C21H42BrNO/c1-3-5-7-9-11-15-19-23(21(24)17-13-14-18-22)20-16-12-10-8-6-

InchiKey: YIOIJYTYHHPOHU-UHFFFAOYSA-N

Formula: C21H42BrNO

SMILES: CCCCCCCCN(CCCCCCCC)C(=O)CCCCBr

Mol. weight [g/mol]: 404.47

Physical Properties

Property code	Value	Unit	Source
gf	122.12	kJ/mol	Joback Method
hf	-495.49	kJ/mol	Joback Method
hfus	60.05	kJ/mol	Joback Method
hvap	77.56	kJ/mol	Joback Method
log10ws	-7.39		Crippen Method
logp	7.101		Crippen Method
mcvol	335.800	ml/mol	McGowan Method
pc	1037.90	kPa	Joback Method
rinpol	2661.00		NIST Webbook
rinpol	2661.00		NIST Webbook
tb	812.35	K	Joback Method
tc	997.12	K	Joback Method
tf	468.63	K	Joback Method
vc	1.298	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1035.54	J/mol×K	812.35	Joback Method
cpg	1054.83	J/mol×K	843.14	Joback Method
cpg	1073.13	J/mol×K	873.94	Joback Method
cpg	1090.50	J/mol×K	904.73	Joback Method
cpg	1106.98	J/mol×K	935.53	Joback Method
cpg	1122.63	J/mol×K	966.32	Joback Method
cpg	1137.50	J/mol×K	997.12	Joback Method

Sources

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=U308265&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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