Propanamide, N,N-dioctyl-2-bromo-

Inchi: InChI=1S/C19H38BrNO/c1-4-6-8-10-12-14-16-21(19(22)18(3)20)17-15-13-11-9-7-5-2/h1
InchiKey: JPHHIXAODKPZBJ-UHFFFAOYSA-N
Formula: C19H38BrNO
SMILES: CCCCCCCCN(CCCCCCCC)C(=O)C(C)Br
Mol. weight [g/mol]: 376.42

Physical Properties

Property code	Value	Unit	Source
gf	102.84	kJ/mol	Joback Method
hf	-459.49	kJ/mol	Joback Method
hfus	51.35	kJ/mol	Joback Method
hvap	72.72	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	6.319		Crippen Method
mcvol	307.620	ml/mol	McGowan Method
pc	1185.79	kPa	Joback Method
rinpol	2346.00		NIST Webbook
rinpol	2346.00		NIST Webbook
tb	766.15	K	Joback Method
tc	947.59	K	Joback Method
tf	431.09	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	914.78	J/mol×K	766.15	Joback Method
cpg	933.37	J/mol×K	796.39	Joback Method
cpg	951.01	J/mol×K	826.63	Joback Method
cpg	967.76	J/mol×K	856.87	Joback Method
cpg	983.65	J/mol×K	887.11	Joback Method
cpg	998.73	J/mol×K	917.35	Joback Method
cpg	1013.06	J/mol×K	947.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308378&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