Benzamide, 4-bromo-N-ethyl-N-heptyl-

Inchi: InChI=1S/C16H24BrNO/c1-3-5-6-7-8-13-18(4-2)16(19)14-9-11-15(17)12-10-14/h9-12H,3
InchiKey: MPXJOGDHIAQTOI-UHFFFAOYSA-N
Formula: C16H24BrNO
SMILES: CCCCCCCN(CC)C(=O)c1ccc(Br)cc1
Mol. weight [g/mol]: 326.27

Physical Properties

Property code	Value	Unit	Source
gf	182.80	kJ/mol	Joback Method
hf	-167.23	kJ/mol	Joback Method
hfus	40.75	kJ/mol	Joback Method
hvap	69.37	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	4.882		Crippen Method
mcvol	241.590	ml/mol	McGowan Method
pc	1877.28	kPa	Joback Method
rinpol	2457.00		NIST Webbook
rinpol	2457.00		NIST Webbook
tb	729.61	K	Joback Method
tc	935.65	K	Joback Method
tf	451.22	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.77	J/mol×K	729.61	Joback Method
cpg	672.82	J/mol×K	763.95	Joback Method
cpg	687.86	J/mol×K	798.29	Joback Method
cpg	701.98	J/mol×K	832.63	Joback Method
cpg	715.22	J/mol×K	866.97	Joback Method
cpg	727.64	J/mol×K	901.31	Joback Method
cpg	739.31	J/mol×K	935.65	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=U415457&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