Pentanamide, n-heptyl-n-octyl-5-bromo-

Inchi: InChI=1S/C20H40BrNO/c1-3-5-7-9-11-15-19-22(18-14-10-8-6-4-2)20(23)16-12-13-17-21
InchiKey: CYUAWCDYVRDWMX-UHFFFAOYSA-N
Formula: C20H40BrNO
SMILES: CCCCCCCCN(CCCCCCC)C(=O)CCCCBr
Mol. weight [g/mol]: 390.45

Physical Properties

Property code	Value	Unit	Source
af	1.0215		Cheméo Relay (1.0)
hf	-574.18	kJ/mol	Cheméo Relay (1.0)
hfus	57.46	kJ/mol	Joback Method
hvap	98.18	kJ/mol	Cheméo Relay (1.0)
ie	8.52	eV	Cheméo Relay (1.0)
log10ws	-5.92		Cheméo Relay (1.0)
logp	6.711		Crippen Method
mcvol	321.710	ml/mol	McGowan Method
pc	1105.21	kPa	Joback Method
rinpol	2562.00		NIST Webbook
tb	633.44	K	Cheméo Relay (1.0)
tc	824.25	K	Cheméo Relay (1.0)
tf	302.53	K	Cheméo Relay (1.0)
vc	1.204	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	974.49	J/mol×K	789.47	Joback Method
cpg	993.34	J/mol×K	819.81	Joback Method
cpg	1011.23	J/mol×K	850.16	Joback Method
cpg	1028.22	J/mol×K	880.50	Joback Method
cpg	1044.36	J/mol×K	910.84	Joback Method
cpg	1059.68	J/mol×K	941.18	Joback Method
cpg	1074.25	J/mol×K	971.53	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308264&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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