1-Naphthamide, N-butyl-N-heptyl-

Inchi: InChI=1S/C22H31NO/c1-3-5-7-8-11-18-23(17-6-4-2)22(24)21-16-12-14-19-13-9-10-15-2
InchiKey: YKXUMSNMIRCEJY-UHFFFAOYSA-N
Formula: C22H31NO
SMILES: CCCCCCCN(CCCC)C(=O)c1cccc2ccccc12
Mol. weight [g/mol]: 325.49

Physical Properties

Property code	Value	Unit	Source
gf	325.65	kJ/mol	Joback Method
hf	-126.33	kJ/mol	Joback Method
hfus	48.03	kJ/mol	Joback Method
hvap	77.93	kJ/mol	Joback Method
log10ws	-7.19		Crippen Method
logp	6.052		Crippen Method
mcvol	289.170	ml/mol	McGowan Method
pc	1363.65	kPa	Joback Method
rinpol	3121.00		NIST Webbook
rinpol	3121.00		NIST Webbook
tb	819.71	K	Joback Method
tc	1024.43	K	Joback Method
tf	491.74	K	Joback Method
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.58	J/mol×K	819.71	Joback Method
cpg	904.20	J/mol×K	853.83	Joback Method
cpg	920.78	J/mol×K	887.95	Joback Method
cpg	936.41	J/mol×K	922.07	Joback Method
cpg	951.19	J/mol×K	956.19	Joback Method
cpg	965.18	J/mol×K	990.31	Joback Method
cpg	978.49	J/mol×K	1024.43	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=U415719&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