N-(3-methylphenyl)-1-naphthamide

Other names: 1-Naphthalenecarboxamide, N-(3-methylphenyl)-
Inchi: InChI=1S/C18H15NO/c1-13-6-4-9-15(12-13)19-18(20)17-11-5-8-14-7-2-3-10-16(14)17/h2
InchiKey: ZQIBGFUTQCVROE-UHFFFAOYSA-N
Formula: C18H15NO
SMILES: Cc1cccc(NC(=O)c2cccc3ccccc23)c1
Mol. weight [g/mol]: 261.32

Physical Properties

Property code	Value	Unit	Source
hf	54.55	kJ/mol	Cheméo Relay (1.0)
hfus	33.40	kJ/mol	Joback Method
ie	7.75	eV	Cheméo Relay (1.0)
log10ws	-5.20		Cheméo Relay (1.0)
logp	4.401		Crippen Method
mcvol	209.050	ml/mol	McGowan Method
rinpol	2543.00		NIST Webbook
tb	684.92	K	Cheméo Relay (1.0)
tf	431.13	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.99	J/mol×K	797.58	Joback Method
cpg	595.23	J/mol×K	839.65	Joback Method
cpg	608.31	J/mol×K	881.72	Joback Method
cpg	620.36	J/mol×K	923.80	Joback Method
cpg	631.50	J/mol×K	965.87	Joback Method
cpg	641.86	J/mol×K	1007.94	Joback Method
cpg	651.58	J/mol×K	1050.01	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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=C301822811&Units=SI

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point