

Butanamide, N-(1-naphthyl)-2,2,3,3,4,4,4-heptafluoro-

Inchi: InChI=1S/C14H8F7NO/c15-12(16,13(17,18)14(19,20)21)11(23)22-10-7-3-5-8-4-1-2-6-9(8)
InchiKey: VERASNSGCMSQDX-UHFFFAOYSA-N
Formula: C14H8F7NO
SMILES: O=C(Nc1cccc2ccccc12)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 339.21

Physical Properties

Property code	Value	Unit	Source
gf	-1118.25	kJ/mol	Joback Method
hf	-1374.29	kJ/mol	Joback Method
hfus	28.70	kJ/mol	Joback Method
hvap	54.91	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	4.611		Crippen Method
mcvol	188.840	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
rinpol	1575.00		NIST Webbook
rinpol	1575.00		NIST Webbook
tb	659.60	K	Joback Method
tc	856.89	K	Joback Method
tf	433.16	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.27	J/mol×K	659.60	Joback Method
cpg	536.78	J/mol×K	692.48	Joback Method
cpg	547.27	J/mol×K	725.36	Joback Method
cpg	556.84	J/mol×K	758.24	Joback Method
cpg	565.60	J/mol×K	791.13	Joback Method
cpg	573.64	J/mol×K	824.01	Joback Method
cpg	581.09	J/mol×K	856.89	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=U307283&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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