Butanamide, N-(3-methylphenyl)-2,2,3,3,4,4,4-heptafluoro-

Inchi: InChI=1S/C11H8F7NO/c1-6-3-2-4-7(5-6)19-8(20)9(12,13)10(14,15)11(16,17)18/h2-5H,1
InchiKey: IMSZHAVHIOIFSQ-UHFFFAOYSA-N
Formula: C11H8F7NO
SMILES: Cc1cccc(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1
Mol. weight [g/mol]: 303.18

Physical Properties

Property code	Value	Unit	Source
gf	-1250.16	kJ/mol	Joback Method
hf	-1503.44	kJ/mol	Joback Method
hfus	23.91	kJ/mol	Joback Method
hvap	46.59	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.766		Crippen Method
mcvol	166.030	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
rinpol	1241.00		NIST Webbook
rinpol	1241.00		NIST Webbook
tb	571.98	K	Joback Method
tc	754.21	K	Joback Method
tf	366.65	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.34	J/mol×K	571.98	Joback Method
cpg	450.50	J/mol×K	602.35	Joback Method
cpg	461.70	J/mol×K	632.72	Joback Method
cpg	472.02	J/mol×K	663.09	Joback Method
cpg	481.50	J/mol×K	693.46	Joback Method
cpg	490.22	J/mol×K	723.83	Joback Method
cpg	498.23	J/mol×K	754.21	Joback Method

Sources

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=U307276&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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