Heptafluorobutanamide, N-ethyl-N-(3-methylphenyl)-

Inchi: InChI=1S/C13H12F7NO/c1-3-21(9-6-4-5-8(2)7-9)10(22)11(14,15)12(16,17)13(18,19)20/h

InchiKey: BURAUADCMPNCGS-UHFFFAOYSA-N

Formula: C13H12F7NO

SMILES: CCN(C(=O)C(F)(F)C(F)(F)C(F)(F)F)c1cccc(C)c1

Mol. weight [g/mol]: 331.23

Physical Properties

Property code	Value	Unit	Source
gf	-1211.93	kJ/mol	Joback Method
hf	-1530.66	kJ/mol	Joback Method
hfus	27.02	kJ/mol	Joback Method
hvap	46.65	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.181		Crippen Method
mcvol	194.210	ml/mol	McGowan Method
pc	1815.41	kPa	Joback Method
rinpol	1297.00		NIST Webbook
tb	580.01	K	Joback Method
tc	755.39	K	Joback Method
tf	369.00	K	Joback Method
vc	0.772	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.99	J/mol×K	580.01	Joback Method
cpg	533.98	J/mol×K	609.24	Joback Method
cpg	546.95	J/mol×K	638.47	Joback Method
cpg	558.99	J/mol×K	667.70	Joback Method
cpg	570.14	J/mol×K	696.93	Joback Method
cpg	580.47	J/mol×K	726.16	Joback Method
cpg	590.05	J/mol×K	755.39	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=U308270&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