N,N'-Di-(m-trifluoromethylphenyl)urea

Inchi: InChI=1S/C15H10F6N2O/c16-14(17,18)9-3-1-5-11(7-9)22-13(24)23-12-6-2-4-10(8-12)15
InchiKey: ASUCRFVOBIZQSN-UHFFFAOYSA-N
Formula: C15H10F6N2O
SMILES: O=C(Nc1cccc(C(F)(F)F)c1)Nc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 348.24
CAS: 403-96-3

Physical Properties

Property code	Value	Unit	Source
gf	-832.34	kJ/mol	Joback Method
hf	-1102.61	kJ/mol	Joback Method
hfus	37.36	kJ/mol	Joback Method
hvap	66.98	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	5.368		Crippen Method
mcvol	206.840	ml/mol	McGowan Method
pc	2125.60	kPa	Joback Method
tb	749.29	K	Joback Method
tc	956.43	K	Joback Method
tf	500.32	K	Joback Method
vc	0.822	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.34	J/mol×K	749.29	Joback Method
cpg	605.63	J/mol×K	783.81	Joback Method
cpg	615.97	J/mol×K	818.34	Joback Method
cpg	625.45	J/mol×K	852.86	Joback Method
cpg	634.15	J/mol×K	887.38	Joback Method
cpg	642.16	J/mol×K	921.90	Joback Method
cpg	649.58	J/mol×K	956.43	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=C403963&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume