Trifluoroacetic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C9H4F3NO2/c10-9(11,12)8(14)15-7-3-1-6(5-13)2-4-7/h1-4H
InchiKey: HWKXKPAUJNGARQ-UHFFFAOYSA-N
Formula: C9H4F3NO2
SMILES: N#Cc1ccc(OC(=O)C(F)(F)F)cc1
Mol. weight [g/mol]: 215.13

Physical Properties

Property code	Value	Unit	Source
gf	-554.65	kJ/mol	Joback Method
hf	-681.03	kJ/mol	Joback Method
hfus	18.84	kJ/mol	Joback Method
hvap	54.45	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.026		Crippen Method
mcvol	128.040	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
rinpol	851.00		NIST Webbook
rinpol	851.00		NIST Webbook
tb	609.93	K	Joback Method
tc	823.96	K	Joback Method
tf	371.47	K	Joback Method
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.80	J/mol×K	609.93	Joback Method
cpg	313.57	J/mol×K	645.60	Joback Method
cpg	321.66	J/mol×K	681.27	Joback Method
cpg	329.09	J/mol×K	716.94	Joback Method
cpg	335.91	J/mol×K	752.62	Joback Method
cpg	342.14	J/mol×K	788.29	Joback Method
cpg	347.82	J/mol×K	823.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307654&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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

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