2-Methyl-3-nitrobenzyl alcohol, trifluoroacetate

Inchi: InChI=1S/C10H8F3NO4/c1-6-7(3-2-4-8(6)14(16)17)5-18-9(15)10(11,12)13/h2-4H,5H2,1H
InchiKey: DQGNCAWKFZZYGP-UHFFFAOYSA-N
Formula: C10H8F3NO4
SMILES: Cc1c(COC(=O)C(F)(F)F)cccc1[N+](=O)[O-]
Mol. weight [g/mol]: 263.17

Physical Properties

Property code	Value	Unit	Source
gf	-653.49	kJ/mol	Joback Method
hf	-888.78	kJ/mol	Joback Method
hfus	30.89	kJ/mol	Joback Method
hvap	63.45	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	2.509		Crippen Method
mcvol	158.170	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
rinpol	1467.00		NIST Webbook
rinpol	1467.00		NIST Webbook
tb	687.55	K	Joback Method
tc	907.64	K	Joback Method
tf	473.88	K	Joback Method
vc	0.636	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.97	J/mol×K	687.55	Joback Method
cpg	431.54	J/mol×K	724.23	Joback Method
cpg	441.28	J/mol×K	760.91	Joback Method
cpg	450.23	J/mol×K	797.59	Joback Method
cpg	458.42	J/mol×K	834.28	Joback Method
cpg	465.90	J/mol×K	870.96	Joback Method
cpg	472.70	J/mol×K	907.64	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376202&Units=SI

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