3-Nitrobenzyl alcohol, trifluoroacetate

Inchi: InChI=1S/C9H6F3NO4/c10-9(11,12)8(14)17-5-6-2-1-3-7(4-6)13(15)16/h1-4H,5H2
InchiKey: AUJHIPQYLBWCBG-UHFFFAOYSA-N
Formula: C9H6F3NO4
SMILES: O=C(OCc1cccc([N+](=O)[O-])c1)C(F)(F)F
Mol. weight [g/mol]: 249.14

Physical Properties

Property code	Value	Unit	Source
gf	-652.28	kJ/mol	Joback Method
hf	-856.67	kJ/mol	Joback Method
hfus	28.69	kJ/mol	Joback Method
hvap	60.57	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	2.200		Crippen Method
mcvol	144.080	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
rinpol	1417.00		NIST Webbook
rinpol	1417.00		NIST Webbook
tb	659.69	K	Joback Method
tc	882.80	K	Joback Method
tf	450.09	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.78	J/mol×K	659.69	Joback Method
cpg	383.86	J/mol×K	696.88	Joback Method
cpg	393.10	J/mol×K	734.06	Joback Method
cpg	401.54	J/mol×K	771.25	Joback Method
cpg	409.23	J/mol×K	808.43	Joback Method
cpg	416.21	J/mol×K	845.62	Joback Method
cpg	422.51	J/mol×K	882.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376155&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

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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