4-(Trifluoromethoxy) benzyl alcohol, acetate

Inchi: InChI=1S/C10H9F3O3/c1-7(14)15-6-8-2-4-9(5-3-8)16-10(11,12)13/h2-5H,6H2,1H3
InchiKey: LEOJDDUQYRSCSH-UHFFFAOYSA-N
Formula: C10H9F3O3
SMILES: CC(=O)OCc1ccc(OC(F)(F)F)cc1
Mol. weight [g/mol]: 234.17

Physical Properties

Property code	Value	Unit	Source
hfus	21.11	kJ/mol	Joback Method
hvap	61.37	kJ/mol	Cheméo Relay (1.0)
logp	2.648		Crippen Method
mcvol	146.620	ml/mol	McGowan Method
rinpol	1202.00		NIST Webbook
tb	478.15	K	Cheméo Relay (1.0)
tf	244.12	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.27	J/mol×K	553.15	Joback Method
cpg	364.21	J/mol×K	585.48	Joback Method
cpg	375.47	J/mol×K	617.81	Joback Method
cpg	386.07	J/mol×K	650.15	Joback Method
cpg	396.01	J/mol×K	682.48	Joback Method
cpg	405.32	J/mol×K	714.81	Joback Method
cpg	414.01	J/mol×K	747.14	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C102606995&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point