4-(Trifluoromethyl)phenyl methanol, n-propyl ether

Inchi: InChI=1S/C11H13F3O/c1-2-7-15-8-9-3-5-10(6-4-9)11(12,13)14/h3-6H,2,7-8H2,1H3
InchiKey: XKRKETPJASPHRZ-UHFFFAOYSA-N
Formula: C11H13F3O
SMILES: CCCOCc1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]: 218.22

Physical Properties

Property code	Value	Unit	Source
gf	-542.07	kJ/mol	Joback Method
hf	-774.61	kJ/mol	Joback Method
hfus	20.91	kJ/mol	Joback Method
hvap	41.68	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.632		Crippen Method
mcvol	153.270	ml/mol	McGowan Method
pc	2287.14	kPa	Joback Method
rinpol	1182.00		NIST Webbook
tb	499.74	K	Joback Method
tc	683.95	K	Joback Method
tf	279.09	K	Joback Method
vc	0.605	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.75	J/mol×K	499.74	Joback Method
cpg	367.96	J/mol×K	530.44	Joback Method
cpg	381.42	J/mol×K	561.14	Joback Method
cpg	394.13	J/mol×K	591.85	Joback Method
cpg	406.14	J/mol×K	622.55	Joback Method
cpg	417.47	J/mol×K	653.25	Joback Method
cpg	428.15	J/mol×K	683.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374663&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