2-Trifluoromethylbenzoic acid, 2-propylphenyl ester

Inchi: InChI=1S/C17H15F3O2/c1-2-7-12-8-3-6-11-15(12)22-16(21)13-9-4-5-10-14(13)17(18,19

InchiKey: JCLMAFWHSQVHQZ-UHFFFAOYSA-N

Formula: C17H15F3O2

SMILES: CCCc1ccccc1OC(=O)c1ccccc1C(F)(F)F

Mol. weight [g/mol]: 308.30

Physical Properties

Property code	Value	Unit	Source
gf	-517.69	kJ/mol	Joback Method
hf	-785.97	kJ/mol	Joback Method
hfus	31.70	kJ/mol	Joback Method
hvap	64.72	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	4.877		Crippen Method
mcvol	215.620	ml/mol	McGowan Method
pc	1910.24	kPa	Joback Method
rinpol	1889.00		NIST Webbook
tb	722.55	K	Joback Method
tc	936.63	K	Joback Method
tf	435.58	K	Joback Method
vc	0.839	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.42	J/mol×K	722.55	Joback Method
cpg	610.91	J/mol×K	758.23	Joback Method
cpg	624.30	J/mol×K	793.91	Joback Method
cpg	636.68	J/mol×K	829.59	Joback Method
cpg	648.08	J/mol×K	865.27	Joback Method
cpg	658.58	J/mol×K	900.95	Joback Method
cpg	668.22	J/mol×K	936.63	Joback Method

Sources

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=U355156&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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