3-Trifluoromethylcinnamic acid, phenyl ester

Inchi: InChI=1S/C16H11F3O2/c17-16(18,19)13-6-4-5-12(11-13)9-10-15(20)21-14-7-2-1-3-8-14
InchiKey: IUBRFAFYCVQGIO-MDZDMXLPSA-N
Formula: C16H11F3O2
SMILES: O=C(C=Cc1cccc(C(F)(F)F)c1)Oc1ccccc1
Mol. weight [g/mol]: 292.25

Physical Properties

Property code	Value	Unit	Source
gf	-436.26	kJ/mol	Joback Method
hf	-636.64	kJ/mol	Joback Method
hfus	29.70	kJ/mol	Joback Method
hvap	61.79	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.324		Crippen Method
mcvol	197.230	ml/mol	McGowan Method
pc	2214.53	kPa	Joback Method
rinpol	1885.90		NIST Webbook
tb	698.85	K	Joback Method
tc	923.57	K	Joback Method
tf	406.71	K	Joback Method
vc	0.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.27	J/mol×K	698.85	Joback Method
cpg	534.96	J/mol×K	736.30	Joback Method
cpg	547.53	J/mol×K	773.76	Joback Method
cpg	559.05	J/mol×K	811.21	Joback Method
cpg	569.61	J/mol×K	848.66	Joback Method
cpg	579.29	J/mol×K	886.12	Joback Method
cpg	588.20	J/mol×K	923.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292634&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