3-Trifluoromethylcinnamic acid, 3,5-difluorophenyl ester

Inchi: InChI=1S/C16H9F5O2/c17-12-7-13(18)9-14(8-12)23-15(22)5-4-10-2-1-3-11(6-10)16(19,2

InchiKey: FEPZWENAXZEKEM-SNAWJCMRSA-N

Formula: C16H9F5O2

SMILES: O=C(C=Cc1cccc(C(F)(F)F)c1)Oc1cc(F)cc(F)c1

Mol. weight [g/mol]: 328.23

Physical Properties

Property code	Value	Unit	Source
gf	-845.14	kJ/mol	Joback Method
hf	-1051.80	kJ/mol	Joback Method
hfus	35.09	kJ/mol	Joback Method
hvap	61.48	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	4.602		Crippen Method
mcvol	200.770	ml/mol	McGowan Method
pc	1984.12	kPa	Joback Method
rinpol	1840.60		NIST Webbook
rinpol	1840.60		NIST Webbook
tb	707.35	K	Joback Method
tc	915.82	K	Joback Method
tf	432.93	K	Joback Method
vc	0.798	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	534.79	J/mol×K	707.35	Joback Method
cpg	546.96	J/mol×K	742.09	Joback Method
cpg	558.21	J/mol×K	776.84	Joback Method
cpg	568.59	J/mol×K	811.58	Joback Method
cpg	578.16	J/mol×K	846.33	Joback Method
cpg	586.98	J/mol×K	881.07	Joback Method
cpg	595.12	J/mol×K	915.82	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U292633&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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