3-Trifluoromethylcinnamic acid, 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C16H9BrF4O2/c17-13-9-12(18)5-6-14(13)23-15(22)7-4-10-2-1-3-11(8-10)16(19

InchiKey: CEUFNHWVEQWLNR-QPJJXVBHSA-N

Formula: C16H9BrF4O2

SMILES: O=C(C=Cc1cccc(C(F)(F)F)c1)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 389.14

Physical Properties

Property code	Value	Unit	Source
gf	-636.01	kJ/mol	Joback Method
hf	-829.36	kJ/mol	Joback Method
hfus	37.29	kJ/mol	Joback Method
hvap	68.73	kJ/mol	Joback Method
log10ws	-6.44		Crippen Method
logp	5.226		Crippen Method
mcvol	216.500	ml/mol	McGowan Method
pc	2202.08	kPa	Joback Method
rinpol	1981.80		NIST Webbook
rinpol	1981.80		NIST Webbook
tb	774.24	K	Joback Method
tc	1001.23	K	Joback Method
tf	492.14	K	Joback Method
vc	0.843	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	560.19	J/mol×K	774.24	Joback Method
cpg	571.26	J/mol×K	812.07	Joback Method
cpg	581.41	J/mol×K	849.90	Joback Method
cpg	590.73	J/mol×K	887.73	Joback Method
cpg	599.31	J/mol×K	925.56	Joback Method
cpg	607.24	J/mol×K	963.39	Joback Method
cpg	614.60	J/mol×K	1001.23	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292637&Units=SI

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