3-Trifluoromethylcinnamic acid, 5-fluoro-2-nitrophenyl ester

Inchi: InChI=1S/C16H9F4NO4/c17-12-5-6-13(21(23)24)14(9-12)25-15(22)7-4-10-2-1-3-11(8-10

InchiKey: UDVLXOSDJLKVOS-QPJJXVBHSA-N

Formula: C16H9F4NO4

SMILES: O=C(C=Cc1cccc(C(F)(F)F)c1)Oc1cc(F)ccc1[N+](=O)[O-]

Mol. weight [g/mol]: 355.24

Physical Properties

Property code	Value	Unit	Source
gf	-614.78	kJ/mol	Joback Method
hf	-866.45	kJ/mol	Joback Method
hfus	43.37	kJ/mol	Joback Method
hvap	78.89	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	4.372		Crippen Method
mcvol	216.420	ml/mol	McGowan Method
pc	2088.84	kPa	Joback Method
rinpol	2225.40		NIST Webbook
tb	859.92	K	Joback Method
tc	1095.37	K	Joback Method
tf	575.95	K	Joback Method
vc	0.863	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.57	J/mol×K	859.92	Joback Method
cpg	629.63	J/mol×K	899.16	Joback Method
cpg	638.78	J/mol×K	938.40	Joback Method
cpg	647.11	J/mol×K	977.64	Joback Method
cpg	654.72	J/mol×K	1016.89	Joback Method
cpg	661.70	J/mol×K	1056.13	Joback Method
cpg	668.13	J/mol×K	1095.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292639&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