trans-3-Trifluoromethylcinnamic acid, 4-nitrophenyl ester

Inchi: InChI=1S/C16H10F3NO4/c17-16(18,19)12-3-1-2-11(10-12)4-9-15(21)24-14-7-5-13(6-8-1

InchiKey: DLCRQNMBWOSQJF-RUDMXATFSA-N

Formula: C16H10F3NO4

SMILES: O=C(C=Cc1cccc(C(F)(F)F)c1)Oc1ccc([N+](=O)[O-])cc1

Mol. weight [g/mol]: 337.25

Physical Properties

Property code	Value	Unit	Source
gf	-410.34	kJ/mol	Joback Method
hf	-658.87	kJ/mol	Joback Method
hfus	40.68	kJ/mol	Joback Method
hvap	79.04	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	4.232		Crippen Method
mcvol	214.650	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
rinpol	2389.00		NIST Webbook
rinpol	2389.00		NIST Webbook
tb	855.67	K	Joback Method
tc	1098.95	K	Joback Method
tf	562.84	K	Joback Method
vc	0.845	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	613.87	J/mol×K	855.67	Joback Method
cpg	624.49	J/mol×K	896.22	Joback Method
cpg	634.14	J/mol×K	936.76	Joback Method
cpg	642.92	J/mol×K	977.31	Joback Method
cpg	650.95	J/mol×K	1017.86	Joback Method
cpg	658.33	J/mol×K	1058.40	Joback Method
cpg	665.18	J/mol×K	1098.95	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=U307813&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