trans-3-Trifluoromethylcinnamic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C16H9Cl2F3O2/c17-13-6-5-12(9-14(13)18)23-15(22)7-4-10-2-1-3-11(8-10)16(
InchiKey: SYIKQBYNUJFNEK-QPJJXVBHSA-N
Formula: C16H9Cl2F3O2
SMILES: O=C(C=Cc1cccc(C(F)(F)F)c1)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 361.14

Physical Properties

Property code	Value	Unit	Source
gf	-479.38	kJ/mol	Joback Method
hf	-691.06	kJ/mol	Joback Method
hfus	37.32	kJ/mol	Joback Method
hvap	71.89	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	5.631		Crippen Method
mcvol	221.710	ml/mol	McGowan Method
pc	2012.70	kPa	Joback Method
rinpol	2310.00		NIST Webbook
rinpol	2310.00		NIST Webbook
tb	783.67	K	Joback Method
tc	1015.30	K	Joback Method
tf	491.59	K	Joback Method
vc	0.861	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.44	J/mol×K	783.67	Joback Method
cpg	575.36	J/mol×K	822.27	Joback Method
cpg	585.34	J/mol×K	860.88	Joback Method
cpg	594.46	J/mol×K	899.48	Joback Method
cpg	602.80	J/mol×K	938.09	Joback Method
cpg	610.45	J/mol×K	976.69	Joback Method
cpg	617.49	J/mol×K	1015.30	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=U307812&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

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