trans-3-Trifluoromethylcinnamic acid, 4-chlorophenyl ester

Inchi: InChI=1S/C16H10ClF3O2/c17-13-5-7-14(8-6-13)22-15(21)9-4-11-2-1-3-12(10-11)16(18,1

InchiKey: KGEZOYSXBMQTOI-RUDMXATFSA-N

Formula: C16H10ClF3O2

SMILES: O=C(C=Cc1cccc(C(F)(F)F)c1)Oc1ccc(Cl)cc1

Mol. weight [g/mol]: 326.70

Physical Properties

Property code	Value	Unit	Source
gf	-457.82	kJ/mol	Joback Method
hf	-663.85	kJ/mol	Joback Method
hfus	33.51	kJ/mol	Joback Method
hvap	66.84	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	4.978		Crippen Method
mcvol	209.470	ml/mol	McGowan Method
pc	2110.00	kPa	Joback Method
rinpol	2112.00		NIST Webbook
tb	741.26	K	Joback Method
tc	969.54	K	Joback Method
tf	449.15	K	Joback Method
vc	0.811	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.97	J/mol×K	741.26	Joback Method
cpg	556.22	J/mol×K	779.31	Joback Method
cpg	567.43	J/mol×K	817.35	Joback Method
cpg	577.70	J/mol×K	855.40	Joback Method
cpg	587.09	J/mol×K	893.45	Joback Method
cpg	595.71	J/mol×K	931.49	Joback Method
cpg	603.64	J/mol×K	969.54	Joback Method

Sources

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=U307808&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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