trans-3-Trifluoromethylcinnamic acid, 4-methoxyphenyl ester

Inchi: InChI=1S/C17H13F3O3/c1-22-14-6-8-15(9-7-14)23-16(21)10-5-12-3-2-4-13(11-12)17(18

InchiKey: RKTVYDVWSGSZRZ-BJMVGYQFSA-N

Formula: C17H13F3O3

SMILES: COc1ccc(OC(=O)C=Cc2cccc(C(F)(F)F)c2)cc1

Mol. weight [g/mol]: 322.28

Physical Properties

Property code	Value	Unit	Source
gf	-542.47	kJ/mol	Joback Method
hf	-800.97	kJ/mol	Joback Method
hfus	33.09	kJ/mol	Joback Method
hvap	67.09	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.333		Crippen Method
mcvol	217.190	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	2182.00		NIST Webbook
tb	749.13	K	Joback Method
tc	968.55	K	Joback Method
tf	452.73	K	Joback Method
vc	0.837	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.43	J/mol×K	749.13	Joback Method
cpg	611.89	J/mol×K	785.70	Joback Method
cpg	624.29	J/mol×K	822.27	Joback Method
cpg	635.68	J/mol×K	858.84	Joback Method
cpg	646.13	J/mol×K	895.41	Joback Method
cpg	655.70	J/mol×K	931.98	Joback Method
cpg	664.45	J/mol×K	968.55	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=U307810&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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