trans-(3-Trifluoromethyl)cinnamic acid, 2-adamantyl ester

Inchi: InChI=1S/C20H21F3O2/c21-20(22,23)17-3-1-2-12(11-17)4-5-18(24)25-19-15-7-13-6-14(

InchiKey: JKVWNHCROYFDQC-SNAWJCMRSA-N

Formula: C20H21F3O2

SMILES: O=C(C=Cc1cccc(C(F)(F)F)c1)OC1C2CC3CC(C2)CC1C3

Mol. weight [g/mol]: 350.37

Physical Properties

Property code	Value	Unit	Source
gf	-360.26	kJ/mol	Joback Method
hf	-784.17	kJ/mol	Joback Method
hfus	40.47	kJ/mol	Joback Method
hvap	67.71	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	5.087		Crippen Method
mcvol	244.770	ml/mol	McGowan Method
pc	1611.58	kPa	Joback Method
rinpol	2318.70		NIST Webbook
rinpol	2318.70		NIST Webbook
tb	778.84	K	Joback Method
tc	997.37	K	Joback Method
tf	467.19	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.67	J/mol×K	778.84	Joback Method
cpg	806.85	J/mol×K	815.26	Joback Method
cpg	823.82	J/mol×K	851.68	Joback Method
cpg	839.72	J/mol×K	888.10	Joback Method
cpg	854.71	J/mol×K	924.52	Joback Method
cpg	868.94	J/mol×K	960.95	Joback Method
cpg	882.55	J/mol×K	997.37	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=U292261&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