trans-(3-Trifluoromethyl)cinnamic acid, 2-(1-adamantyl)ethyl ester

Inchi: InChI=1S/C22H25F3O2/c23-22(24,25)19-3-1-2-15(11-19)4-5-20(26)27-7-6-21-12-16-8-17(13-21)10-18(9-16)14-21/h1-4,11,16-18H,5-10,12-14H2/b5-4+

InchiKey: XKDTWQBLOXEVMG-SNAWJCMRSA-N

Formula: C22H25F3O2

SMILES: O=C(C=Cc1cccc(C(F)(F)F)c1)OCCC12CC3CC(CC(C3)C1)C2

Mol. weight [g/mol]: 378.43

Physical Properties

Property code	Value	Unit	Source
gf	-341.20	kJ/mol	Joback Method
hf	-789.87	kJ/mol	Joback Method
hfus	38.28	kJ/mol	Joback Method
hvap	71.32	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	5.868		Crippen Method
mcvol	272.950	ml/mol	McGowan Method
pc	1473.62	kPa	Joback Method
rinpol	2485.60		NIST Webbook
rinpol	2485.60		NIST Webbook
tb	829.51	K	Joback Method
tc	1049.22	K	Joback Method
tf	517.87	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	897.91	J/mol×K	829.51	Joback Method
cpg	917.52	J/mol×K	866.13	Joback Method
cpg	936.69	J/mol×K	902.75	Joback Method
cpg	955.67	J/mol×K	939.37	Joback Method
cpg	974.72	J/mol×K	975.99	Joback Method
cpg	994.08	J/mol×K	1012.60	Joback Method
cpg	1014.01	J/mol×K	1049.22	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=U292263&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