

trans-3-(Trifluoromethyl)cinnamic acid, tridecyl ester

Inchi:	InChI=1S/C23H33F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-18-28-22(27)17-16-20-14-13-15-21
InchiKey:	OEPZSYJJQMQUCC-WUKNDPDISA-N
Formula:	C23H33F3O2
SMILES:	CCCCCCCCCCCCOC(=O)C=Cc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	398.50

Physical Properties

Property code	Value	Unit	Source
gf	-489.73	kJ/mol	Joback Method
hf	-1017.65	kJ/mol	Joback Method
hfus	53.79	kJ/mol	Joback Method
hvap	75.10	kJ/mol	Joback Method
log10ws	-8.12		Crippen Method
logp	7.573		Crippen Method
mcvol	319.620	ml/mol	McGowan Method
pc	1022.04	kPa	Joback Method
tb	832.33	K	Joback Method
tc	1023.46	K	Joback Method
tf	459.18	K	Joback Method
vc	1.262	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1002.98	J/molxK	832.33	Joback Method
cpg	1020.36	J/molxK	864.18	Joback Method
cpg	1036.74	J/molxK	896.04	Joback Method
cpg	1052.18	J/molxK	927.89	Joback Method
cpg	1066.73	J/molxK	959.75	Joback Method
cpg	1080.48	J/molxK	991.60	Joback Method
cpg	1093.47	J/molxK	1023.46	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=U299875&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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