

Trans-3-(trifluoromethyl)cinnamic acid, hexyl ester

Inchi:	InChI=1S/C16H19F3O2/c1-2-3-4-5-11-21-15(20)10-9-13-7-6-8-14(12-13)16(17,18)19/h6
InchiKey:	RJHBSTPQTPVUIW-MDZDMXLPSA-N
Formula:	C16H19F3O2
SMILES:	CCCCCOC(=O)/C=C/c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	300.32

Physical Properties

Property code	Value	Unit	Source
hfus	35.66	kJ/mol	Joback Method
ie	9.18	eV	Cheméo Relay (1.0)
log10ws	-5.84		Cheméo Relay (1.0)
logp	4.842		Crippen Method
mcvol	220.990	ml/mol	McGowan Method
pc	1657.84	kPa	Joback Method
rinpol	1813.00		NIST Webbook
rinpol	1813.00		NIST Webbook
tb	582.86	K	Cheméo Relay (1.0)
tf	318.65	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.07	J/mol×K	672.17	Joback Method
cpg	619.14	J/mol×K	703.77	Joback Method
cpg	633.31	J/mol×K	735.37	Joback Method
cpg	646.61	J/mol×K	766.97	Joback Method
cpg	659.11	J/mol×K	798.58	Joback Method
cpg	670.84	J/mol×K	830.18	Joback Method
cpg	681.86	J/mol×K	861.78	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299870&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/35-055-2/Trans-3-trifluoromethyl-cinnamic-acid-hexyl-ester.pdf>

Generated by Cheméo on 2026-07-21 22:55:41.823132389 +0000 UTC m=+185637.665017766.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.