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: CCCCCCOC(=O)C=Cc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 300.32

Physical Properties

Property code	Value	Unit	Source
gf	-548.67	kJ/mol	Joback Method
hf	-873.17	kJ/mol	Joback Method
hfus	35.66	kJ/mol	Joback Method
hvap	59.52	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.842		Crippen Method
mcvol	220.990	ml/mol	McGowan Method
pc	1657.84	kPa	Joback Method
rinpol	1813.00		NIST Webbook
tb	672.17	K	Joback Method
tc	861.78	K	Joback Method
tf	380.29	K	Joback Method
vc	0.871	m3/kmol	Joback Method

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299870&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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

Latest version available from:
https://www.chemeo.com/cid/35-055-2/trans-3-Trifluoromethyl-cinnamic-acid-hexyl-ester.pdf
Generated by Cheméo on 2024-10-12 08:09:45.04790519 +0000 UTC m=+3301447.684874438.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.