

Trans-cinnamamide, n,n-diundecyl-3-trifluoromethyl-

Inchi: InChI=1S/C32H52F3NO/c1-3-5-7-9-11-13-15-17-19-26-36(27-20-18-16-14-12-10-8-6-4-2)
InchiKey: ZCVVTCJFCQUZGD-OCOZRVBESA-N
Formula: C32H52F3NO
SMILES: CCCCCCCCCCN(CCCCCCCCCCCC)C(=O)/C=C/c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 523.77

Physical Properties

Property code	Value	Unit	Source
hfus	78.94	kJ/mol	Joback Method
ie	8.98	eV	Cheméo Relay (1.0)
logp	10.609		Crippen Method
mcvol	450.540	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1585.17	J/mol×K	1028.27	Joback Method
cpg	1609.33	J/mol×K	1069.62	Joback Method
cpg	1632.25	J/mol×K	1110.97	Joback Method
cpg	1654.15	J/mol×K	1152.33	Joback Method
cpg	1675.25	J/mol×K	1193.68	Joback Method
cpg	1695.79	J/mol×K	1235.03	Joback Method
cpg	1715.99	J/mol×K	1276.38	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=U308079&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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