Tridecyl pentafluoropropionate

Other names: Tridecyl pentafluoropropionate
Inchi: InChI=1S/C16H27F5O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-23-14(22)15(17,18)16(19,20)21/
InchiKey: WGTROCTZHUYVJI-UHFFFAOYSA-N
Formula: C16H27F5O2
SMILES: CCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 346.38

Physical Properties

Property code	Value	Unit	Source
af	0.8165		Cheméo Relay (1.0)
hf	-1695.22	kJ/mol	Cheméo Relay (1.0)
hfus	40.55	kJ/mol	Joback Method
hvap	80.03	kJ/mol	Cheméo Relay (1.0)
ie	10.54	eV	Cheméo Relay (1.0)
log10ws	-6.68		Cheméo Relay (1.0)
logp	6.038		Crippen Method
mcvol	252.590	ml/mol	McGowan Method
pc	1193.17	kPa	Joback Method
rinpol	1533.00		NIST Webbook
rinpol	1534.50		NIST Webbook
rinpol	1534.50		NIST Webbook
rinpol	1533.00		NIST Webbook
tb	512.35	K	Cheméo Relay (1.0)
tc	630.76	K	Cheméo Relay (1.0)
tf	265.89	K	Cheméo Relay (1.0)
vc	0.966	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.36	J/mol×K	631.66	Joback Method
cpg	736.59	J/mol×K	657.50	Joback Method
cpg	752.06	J/mol×K	683.35	Joback Method
cpg	766.79	J/mol×K	709.19	Joback Method

cpg	780.81	J/mol×K	735.03	Joback Method
cpg	794.15	J/mol×K	760.87	Joback Method
cpg	806.84	J/mol×K	786.72	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C959261224&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/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization 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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume