Octadecyl pentafluoropropionate

Other names: Octadecyl pentafluoropropionate
Inchi: InChI=1S/C21H37F5O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-28-19(27)20(22
InchiKey: KNCMVQBRQJKYNM-UHFFFAOYSA-N
Formula: C21H37F5O2
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 416.51

Physical Properties

Property code	Value	Unit	Source
af	0.9957		Cheméo Relay (1.0)
hf	-1793.70	kJ/mol	Cheméo Relay (1.0)
hfus	53.51	kJ/mol	Joback Method
hvap	100.54	kJ/mol	Cheméo Relay (1.0)
ie	10.58	eV	Cheméo Relay (1.0)
log10ws	-8.12		Cheméo Relay (1.0)
logp	7.989		Crippen Method
mcvol	323.040	ml/mol	McGowan Method
pc	877.91	kPa	Joback Method
rinpol	2008.00		NIST Webbook
rinpol	2054.00		NIST Webbook
rinpol	2011.00		NIST Webbook
rinpol	2008.00		NIST Webbook
rinpol	2011.00		NIST Webbook
ripol	2097.00		NIST Webbook
tb	570.18	K	Cheméo Relay (1.0)
tc	688.12	K	Cheméo Relay (1.0)
tf	291.27	K	Cheméo Relay (1.0)
vc	1.236	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1009.73	J/mol×K	746.06	Joback Method
cpg	1028.45	J/mol×K	774.05	Joback Method

cpg	1046.22	J/mol×K	802.04	Joback Method
cpg	1063.07	J/mol×K	830.03	Joback Method
cpg	1079.07	J/mol×K	858.02	Joback Method
cpg	1094.24	J/mol×K	886.01	Joback Method
cpg	1108.65	J/mol×K	914.00	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C959261257&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

Cheméo Relay (1.0):

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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