

Heptadecyl pentafluoropropionate

Other names:	Heptadecyl pentafluoropropionate
Inchi:	InChI=1S/C20H35F5O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-27-18(26)19(21,22)
InchiKey:	YUZPMKBRUISFHZ-UHFFFAOYSA-N
Formula:	C20H35F5O2
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	402.49

Physical Properties

Property code	Value	Unit	Source
af	0.9601		Cheméo Relay (1.0)
hf	-1773.71	kJ/mol	Cheméo Relay (1.0)
hfus	50.91	kJ/mol	Joback Method
hvap	96.34	kJ/mol	Cheméo Relay (1.0)
ie	10.56	eV	Cheméo Relay (1.0)
log10ws	-7.84		Cheméo Relay (1.0)
logp	7.599		Crippen Method
mcvol	308.950	ml/mol	McGowan Method
pc	930.07	kPa	Joback Method
rinpol	1909.00		NIST Webbook
rinpol	1912.70		NIST Webbook
rinpol	1912.70		NIST Webbook
rinpol	1909.00		NIST Webbook
tb	559.16	K	Cheméo Relay (1.0)
tc	677.49	K	Cheméo Relay (1.0)
tf	286.98	K	Cheméo Relay (1.0)
vc	1.182	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	949.84	J/mol×K	723.18	Joback Method
cpg	968.01	J/mol×K	750.54	Joback Method
cpg	985.27	J/mol×K	777.89	Joback Method
cpg	1001.67	J/mol×K	805.25	Joback Method

cpg	1017.24	J/mol×K	832.61	Joback Method
cpg	1032.02	J/mol×K	859.96	Joback Method
cpg	1046.06	J/mol×K	887.32	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=C959218781&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>

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

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