

VERTREL 245

Inchi: InChI=1S/C6F12/c7-1(5(13,14)15)2(8,6(16,17)18)4(11,12)3(1,9)10
InchiKey: RBTROQHBNLSUTL-UHFFFAOYSA-N
Formula: C6F12
SMILES: FC(F)(F)C1(F)C(F)(F)C(F)(F)C1(F)C(F)(F)F
Mol. weight [g/mol]: 300.04

Physical Properties

Property code	Value	Unit	Source
af	0.4033		Cheméo Relay (1.0)
hf	-2509.43	kJ/mol	Cheméo Relay (1.0)
hfus	7.48	kJ/mol	Joback Method
hvap	32.32	kJ/mol	Cheméo Relay (1.0)
logp	3.812		Crippen Method
mcvol	105.780	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
tb	318.15	K	NCMS SOLV-DB
tc	477.46	K	Cheméo Relay (1.0)
tf	241.15	K	NCMS SOLV-DB
vc	0.452	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
pvap	50.26	kPa	298.15	NCMS SOLV-DB

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K

Coeff. A	-2.15930e+02
Coeff. B	2.19640e+00
Coeff. C	-2.98100e-03
Coeff. D	1.44800e-06
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

NCMS SOLV-DB:	http://solvdb.ncms.org/common01.idc?solvno=DUPNTV245
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):	
Cheméo Relay (1.0, beta):	

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
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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