2,2,3-trichloro-1,1,1,3,4,4,4-heptafluorobutane

Inchi: InChI=1S/C4Cl3F7/c5-1(6,3(9,10)11)2(7,8)4(12,13)14
InchiKey: ZPGMWBFCBUKITA-UHFFFAOYSA-N
Formula: C4Cl3F7
SMILES: FC(F)(F)C(F)(Cl)C(Cl)(Cl)C(F)(F)F
Mol. weight [g/mol]: 287.39
CAS: 335-44-4

Physical Properties

Property code	Value	Unit	Source
af	0.3467		Cheméo Relay (1.0)
hf	-1629.94	kJ/mol	Cheméo Relay (1.0)
hfus	10.61	kJ/mol	Joback Method
hvap	34.03	kJ/mol	Cheméo Relay (1.0)
ie	11.79	eV	Cheméo Relay (1.0)
log10ws	-4.77		Cheméo Relay (1.0)
logp	4.190		Crippen Method
mcvol	116.330	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
tb	362.26	K	Cheméo Relay (1.0)
tc	534.00	K	Cheméo Relay (1.0)
tf	234.55	K	Cheméo Relay (1.0)
vc	0.455	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.48	J/mol×K	385.18	Joback Method
cpg	238.77	J/mol×K	413.12	Joback Method
cpg	247.18	J/mol×K	441.06	Joback Method
cpg	254.74	J/mol×K	469.00	Joback Method
cpg	261.50	J/mol×K	496.95	Joback Method
cpg	267.52	J/mol×K	524.89	Joback Method
cpg	272.86	J/mol×K	552.83	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.36283e+01
Coeff. B	-2.75994e+03
Coeff. C	-6.48280e+01
Temperature range (K), min.	271.71
Temperature range (K), max.	396.68

Sources

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
pvap: Vapor pressure

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