Perfluoro-2,7-dimethyloctane

Inchi: InChI=1S/C10F22/c11-1(7(21,22)23,8(24,25)26)3(13,14)5(17,18)6(19,20)4(15,16)2(12,9(
InchiKey: OBAVAMUHCSFDSY-UHFFFAOYSA-N
Formula: C10F22
SMILES: FC(F)(F)C(F)(C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 538.07
CAS: 3021-63-4

Physical Properties

Property code	Value	Unit	Source
chl	-3184.60	kJ/mol	NIST Webbook
gf	-4224.10	kJ/mol	Joback Method
hf	-4639.10 ± 8.80	kJ/mol	NIST Webbook
hfl	-4687.90 ± 8.70	kJ/mol	NIST Webbook
hfus	15.28	kJ/mol	Joback Method
hvap	48.80 ± 1.10	kJ/mol	NIST Webbook
log10ws	-7.85		Crippen Method
logp	7.193		Crippen Method
mcvol	190.700	ml/mol	McGowan Method
pc	1127.59	kPa	Joback Method
tb	379.84	K	Joback Method
tc	482.36	K	Joback Method
tf	239.64	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.89	J/mol×K	379.84	Joback Method
cpg	513.97	J/mol×K	396.93	Joback Method
cpg	528.19	J/mol×K	414.01	Joback Method
cpg	541.59	J/mol×K	431.10	Joback Method
cpg	554.18	J/mol×K	448.19	Joback Method
cpg	566.00	J/mol×K	465.27	Joback Method
cpg	577.08	J/mol×K	482.36	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56387e+01
Coeff. B	-3.93912e+03
Coeff. C	-5.71180e+01
Temperature range (K), min.	313.72
Temperature range (K), max.	438.55

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3021634&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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