

OCTAFLUORONAPHTHALENE

Other names:	Naphthalene, octafluoro- Perfluoronaphthalene
Inchi:	InChI=1S/C10F8/c11-3-1-2(5(13)9(17)7(3)15)6(14)10(18)8(16)4(1)12
InchiKey:	JDCMOHAFGDQQJX-UHFFFAOYSA-N
Formula:	C10F8
SMILES:	Fc1c(F)c(F)c2c(F)c(F)c(F)c(F)c2c1F
Mol. weight [g/mol]:	272.09
CAS:	313-72-4

Physical Properties

Property code	Value	Unit	Source
af	0.5044		Cheméo Relay (1.0)
gf	-1383.14	kJ/mol	Joback Method
hf	-1063.98	kJ/mol	Cheméo Relay (1.0)
hfus	34.24	kJ/mol	Joback Method
ie	8.85	eV	NIST Webbook
ie	8.87 ± 0.02	eV	NIST Webbook
ie	8.85	eV	NIST Webbook
ie	8.90 ± 0.05	eV	NIST Webbook
logp	3.953		Crippen Method
mcvol	122.700	ml/mol	McGowan Method
pc	2306.95	kPa	Joback Method
rinpol	1103.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	186.73		NIST Webbook
rinpol	189.20		NIST Webbook
rinpol	186.73		NIST Webbook
ripol	162.99		NIST Webbook
ripol	162.99		NIST Webbook
tb	482.00	K	KDB
tc	673.10	K	KDB
tf	360.60	K	KDB
vc	0.499	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.09	J/mol×K	507.86	Joback Method
cpg	281.81	J/mol×K	535.48	Joback Method
cpg	288.24	J/mol×K	563.10	Joback Method
cpg	294.40	J/mol×K	590.73	Joback Method
cpg	300.29	J/mol×K	618.35	Joback Method
cpg	305.92	J/mol×K	645.97	Joback Method
cpg	311.29	J/mol×K	673.59	Joback Method
hfust	17.55	kJ/mol	358.80	NIST Webbook
hsubt	79.40 ± 2.50	kJ/mol	308.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.22011e+01
Coeff. B	-2.59380e+03
Coeff. C	-1.42084e+02
Temperature range (K), min.	359.80
Temperature range (K), max.	518.56

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C313724&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1708.mol

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor 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

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