

Dodecane, 1-fluoro-

Other names:	1-Fluorododecane Dodecyl fluoride n-Dodecyl fluoride
Inchi:	InChI=1S/C12H25F/c1-2-3-4-5-6-7-8-9-10-11-12-13/h2-12H2,1H3
InchiKey:	YHYBNVZCQIDLSQ-UHFFFAOYSA-N
Formula:	C12H25F
SMILES:	CCCCCCCCCCCCF
Mol. weight [g/mol]:	188.33
CAS:	334-68-9

Physical Properties

Property code	Value	Unit	Source
chl	-7921.60 ± 0.59	kJ/mol	NIST Webbook
gf	-144.65	kJ/mol	Joback Method
hf	-489.22 ± 0.61	kJ/mol	NIST Webbook
hfl	-553.19 ± 0.59	kJ/mol	NIST Webbook
hfus	29.92	kJ/mol	Joback Method
hvap	63.97 ± 0.16	kJ/mol	NIST Webbook
hvap	64.00 ± 0.20	kJ/mol	NIST Webbook
log10ws	-4.70		Crippen Method
logp	4.877		Crippen Method
mcvol	181.710	ml/mol	McGowan Method
pc	1714.61	kPa	Joback Method
tb	473.23	K	Joback Method
tc	627.12	K	Joback Method
tf	225.59	K	Joback Method
vc	0.726	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	414.95	J/mol×K	473.23	Joback Method
cpg	430.99	J/mol×K	498.88	Joback Method
cpg	446.46	J/mol×K	524.53	Joback Method

cpg	461.36	J/mol×K	550.18	Joback Method
cpg	475.70	J/mol×K	575.82	Joback Method
cpg	489.51	J/mol×K	601.47	Joback Method
cpg	502.80	J/mol×K	627.12	Joback Method
hvapt	56.20	kJ/mol	453.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.34438e+01
Coeff. B	-3.86640e+03
Coeff. C	-7.96360e+01
Temperature range (K), min.	373.52
Temperature range (K), max.	555.07

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C334689&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/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

hvapt:	Enthalpy of vaporization at a given temperature
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

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