DOTETRACONTAFLUOROICOSANE

Other names: dotetracontafluoroeicosane
eicosane, dotetracontafluoro-
perfluoroeicosane
Inchi: InChI=1S/C20F42/c21-1(22,3(25,26)5(29,30)7(33,34)9(37,38)11(41,42)13(45,46)15(49,5
InchiKey: WSXNCJNDCDTRSA-UHFFFAOYSA-N
Formula: C20F42
SMILES: FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F
Mol. weight [g/mol]: 1038.14

Physical Properties

Property code	Value	Unit	Source
af	0.9789		Cheméo Relay (1.0)
gf	-8007.70	kJ/mol	Joback Method
hf	-8645.09	kJ/mol	Cheméo Relay (1.0)
hfus	50.30	kJ/mol	Applications of Correlation Gas Chromatography and Transpiration Studies for the Evaluation of the Vaporization and Sublimation Enthalpies of Some Perfluorinated Hydrocarbons
hvap	81.35	kJ/mol	Cheméo Relay (1.0)
ie	12.22	eV	Cheméo Relay (1.0)
logp	13.546		Crippen Method
mcvol	367.000	ml/mol	McGowan Method
pc	462.88	kPa	Joback Method
tb	571.26	K	Cheméo Relay (1.0)
tc	613.12	K	Cheméo Relay (1.0)
tf	437.90 ± 0.50	K	NIST Webbook
tf	437.90 ± 0.20	K	NIST Webbook
tf	435.60 ± 0.20	K	NIST Webbook
tf	443.20 ± 0.20	K	NIST Webbook
vc	1.697	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1211.64	J/mol×K	561.74	Joback Method
cpg	1300.76	J/mol×K	699.59	Joback Method
cpg	1289.88	J/mol×K	676.62	Joback Method
cpg	1277.60	J/mol×K	653.64	Joback Method
cpg	1263.77	J/mol×K	630.67	Joback Method
cpg	1248.26	J/mol×K	607.69	Joback Method
cpg	1230.93	J/mol×K	584.72	Joback Method
hfust	80.33	kJ/mol	437.90	NIST Webbook
hfust	80.33	kJ/mol	437.90	NIST Webbook
hfust	11.25	kJ/mol	202.90	NIST Webbook
hfust	0.67	kJ/mol	149.50	NIST Webbook
sfust	183.44	J/mol×K	437.90	NIST Webbook
sfust	55.45	J/mol×K	202.90	NIST Webbook
sfust	4.48	J/mol×K	149.50	NIST Webbook

Sources

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):

Applications of Correlation Gas Chromatography and Transpiration Studies for the Evaluation of the Vaporization and Sublimation Enthalpies of Some Perfluorinated Hydrocarbons: https://www.doi.org/10.1021/je300504f

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C37589574&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume