

ALPHA,ALPHA,ALPHA,2,3,5,6-HEPTAFLUORO-P-

Inchi: InChI=1S/C8H3F7/c1-2-4(9)6(11)3(8(13,14)15)7(12)5(2)10/h1H3
InchiKey: JBZHWNXMZBYBXDQ-UHFFFAOYSA-N
Formula: C8H3F7
SMILES: Cc1c(F)c(F)c(C(F)(F)F)c(F)c1F
Mol. weight [g/mol]: 232.10

Physical Properties

Property code	Value	Unit	Source
af	0.4292		Cheméo Relay (1.0)
hf	-1234.90	kJ/mol	Cheméo Relay (1.0)
hfus	22.72	kJ/mol	Joback Method
hvap	40.00	kJ/mol	Cheméo Relay (1.0)
ie	9.67	eV	Cheméo Relay (1.0)
logp	3.570		Crippen Method
mcvol	112.210	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
tb	417.20	K	NIST Webbook
tc	566.46	K	Cheméo Relay (1.0)
tf	219.02	K	Cheméo Relay (1.0)
vc	0.438	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.02	J/mol×K	425.68	Joback Method
cpg	249.12	J/mol×K	452.20	Joback Method
cpg	256.85	J/mol×K	478.73	Joback Method
cpg	264.22	J/mol×K	505.25	Joback Method
cpg	271.25	J/mol×K	531.77	Joback Method
cpg	277.93	J/mol×K	558.30	Joback Method
cpg	284.29	J/mol×K	584.82	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C778358&Units=SI>

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
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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