Heptafluorobutyric acid, n-pentyl ester

Other names:	2,2,3,3,4,4,4-Heptafluoro-butyric acid pentyl ester
	Butanoic acid, heptafluoro, pentyl ester
	Pentyl heptafluorobutanoate
	Heptafluorobutyric acid, pentyl ester
	Pentyl heptafluorobutyrate
Inchi:	InChI=1S/C9H11F7O2/c1-2-3-4-5-18-6(17)7(10,11)8(12,13)9(14,15)16/h2-5H2,1H3
InchiKey:	RLAQTSYDDYVBHR-UHFFFAOYSA-N
Formula:	C9H11F7O2
SMILES:	CCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	284.17
CAS:	425-26-3

Physical Properties

Property code	Value	Unit	Source
gf	-1564.17	kJ/mol	Joback Method
hf	-1872.91	kJ/mol	Joback Method
hfus	21.17	kJ/mol	Joback Method
hvap	35.18	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.553		Crippen Method
mcvol	157.500	ml/mol	McGowan Method
pc	1900.26	kPa	Joback Method
rinpol	839.00		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	841.00		NIST Webbook
rinpol	839.00		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	829.90		NIST Webbook
rinpol	835.00		NIST Webbook
rinpol	841.00		NIST Webbook
ripol	835.00		NIST Webbook
tb	413.65 ± 2.00	K	NIST Webbook
tc	614.94	K	Joback Method
tf	274.74	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.47	J/mol×K	466.81	Joback Method
cpg	400.80	J/mol×K	491.50	Joback Method
cpg	412.46	J/mol×K	516.19	Joback Method
cpg	423.49	J/mol×K	540.88	Joback Method
cpg	433.91	J/mol×K	565.57	Joback Method
cpg	443.74	J/mol×K	590.25	Joback Method
cpg	453.02	J/mol×K	614.94	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C425263&Units=SI
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

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
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
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