Octyl pentafluoropropionate

Inchi: InChI=1S/C11H17F5O2/c1-2-3-4-5-6-7-8-18-9(17)10(12,13)11(14,15)16/h2-8H2,1H3
InchiKey: ZPVRQKZQZAFDCY-UHFFFAOYSA-N
Formula: C11H17F5O2
SMILES: CCCCCCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 276.24

Physical Properties

Property code	Value	Unit	Source
af	0.6297		Cheméo Relay (1.0)
hf	-1592.65	kJ/mol	Cheméo Relay (1.0)
hfus	27.60	kJ/mol	Joback Method
hvap	57.63	kJ/mol	Cheméo Relay (1.0)
ie	10.64	eV	Cheméo Relay (1.0)
log10ws	-4.95		Cheméo Relay (1.0)
logp	4.088		Crippen Method
mcvol	182.140	ml/mol	McGowan Method
pc	1714.61	kPa	Joback Method
rinpol	1076.60		NIST Webbook
rinpol	1062.00		NIST Webbook
rinpol	1071.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1076.60		NIST Webbook
rinpol	1062.00		NIST Webbook
ripol	1114.00		NIST Webbook
ripol	1120.00		NIST Webbook
tb	442.44	K	Cheméo Relay (1.0)
tc	563.61	K	Cheméo Relay (1.0)
tf	230.62	K	Cheméo Relay (1.0)
vc	0.690	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.85	J/mol×K	517.26	Joback Method

cpg	475.56	J/mol×K	542.77	Joback Method
cpg	488.62	J/mol×K	568.27	Joback Method
cpg	501.04	J/mol×K	593.78	Joback Method
cpg	512.87	J/mol×K	619.28	Joback Method
cpg	524.11	J/mol×K	644.79	Joback Method
cpg	534.79	J/mol×K	670.29	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1867954&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):
Cheméo Relay (1.0, beta):

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
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