1-Heptafluorobutyryloxydecane

Other names:	Decyl heptafluorobutyrate
	Decyl 2,2,3,3,4,4,4-heptafluorobutanoate
	1-Decanol, heptafluorobutyrate
	Decyl perfluorobutyrate
	Decyl heptafluorobutanoate
	Heptafluorobutyric acid, decyl ester
Inchi:	InChI=1S/C14H21F7O2/c1-2-3-4-5-6-7-8-9-10-23-11(22)12(15,16)13(17,18)14(19,20)21/
InchiKey:	FBFAFFNIDITULK-UHFFFAOYSA-N
Formula:	C14H21F7O2
SMILES:	CCCCCCCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	354.30
CAS:	2994-16-3

Physical Properties

Property code	Value	Unit	Source
gf	-1522.07	kJ/mol	Joback Method
hf	-1976.11	kJ/mol	Joback Method
hfus	34.12	kJ/mol	Joback Method
hvap	46.31	kJ/mol	Joback Method
log10ws	-5.84		Crippen Method
logp	5.503		Crippen Method
mcvol	227.950	ml/mol	McGowan Method
pc	1299.53	kPa	Joback Method
rinpol	1298.00		NIST Webbook
rinpol	1301.90		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1298.00		NIST Webbook
ripol	1311.00		NIST Webbook
tb	581.21	K	Joback Method
tc	730.55	K	Joback Method
tf	331.09	K	Joback Method
vc	0.936	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.54	J/mol×K	581.21	Joback Method
cpg	646.44	J/mol×K	606.10	Joback Method
cpg	660.59	J/mol×K	630.99	Joback Method
cpg	674.02	J/mol×K	655.88	Joback Method
cpg	686.75	J/mol×K	680.77	Joback Method
cpg	698.83	J/mol×K	705.66	Joback Method
cpg	710.29	J/mol×K	730.55	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2994163&Units=SI

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