

2-Decanol, heptafluorobutyrate

Inchi:	InChI=1S/C14H21F7O2/c1-3-4-5-6-7-8-9-10(2)23-11(22)12(15,16)13(17,18)14(19,20)21
InchiKey:	RVXVQCAJFIKZHO-UHFFFAOYSA-N
Formula:	C14H21F7O2
SMILES:	CCCCCCCCC(C)OC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	354.30

Physical Properties

Property code	Value	Unit	Source
gf	-1524.51	kJ/mol	Joback Method
hf	-1981.39	kJ/mol	Joback Method
hfus	30.60	kJ/mol	Joback Method
hvap	45.92	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	5.502		Crippen Method
mcvol	227.950	ml/mol	McGowan Method
pc	1307.06	kPa	Joback Method
rinpol	1244.80		NIST Webbook
rinpol	1244.80		NIST Webbook
tb	580.77	K	Joback Method
tc	732.00	K	Joback Method
tf	316.09	K	Joback Method
vc	0.930	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.85	J/mol×K	580.77	Joback Method
cpg	646.99	J/mol×K	605.98	Joback Method
cpg	661.35	J/mol×K	631.18	Joback Method
cpg	674.97	J/mol×K	656.39	Joback Method
cpg	687.87	J/mol×K	681.59	Joback Method
cpg	700.10	J/mol×K	706.80	Joback Method
cpg	711.68	J/mol×K	732.00	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=U352326&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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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