Decyl trifluoroacetate

Other names:	Decyl 2,2,2-trifluoroacetate
	1-Decanol, trifluoroacetate
	Acetic acid, trifluoro-, decyl ester
	1-Trifluoroacetoxydecane
	Trifluoroacetic acid, decyl ester
Inchi:	InChI=1S/C12H21F3O2/c1-2-3-4-5-6-7-8-9-10-17-11(16)12(13,14)15/h2-10H2,1H3
InchiKey:	VOYQYHZKXRAELV-UHFFFAOYSA-N
Formula:	C12H21F3O2
SMILES:	CCCCCCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]:	254.29
CAS:	333-88-0

Physical Properties

Property code	Value	Unit	Source
gf	-765.35	kJ/mol	Joback Method
hf	-1132.89	kJ/mol	Joback Method
hfus	31.45	kJ/mol	Joback Method
hvap	47.72	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	4.233		Crippen Method
mcvol	192.690	ml/mol	McGowan Method
pc	1679.66	kPa	Joback Method
rinpol	1247.20		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1247.20		NIST Webbook
rinpol	1232.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1273.60		NIST Webbook
rinpol	1220.00		NIST Webbook
ripol	1367.00		NIST Webbook
ripol	1367.00		NIST Webbook
tb	544.83	K	Joback Method
tc	702.65	K	Joback Method
tf	301.35	K	Joback Method
vc	0.774	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.45	J/mol×K	544.83	Joback Method
cpg	506.08	J/mol×K	571.13	Joback Method
cpg	520.09	J/mol×K	597.44	Joback Method
cpg	533.48	J/mol×K	623.74	Joback Method
cpg	546.28	J/mol×K	650.04	Joback Method
cpg	558.51	J/mol×K	676.35	Joback Method
cpg	570.18	J/mol×K	702.65	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C333880&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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