2-Decanol, trifluoroacetate

Inchi: InChI=1S/C12H21F3O2/c1-3-4-5-6-7-8-9-10(2)17-11(16)12(13,14)15/h10H,3-9H2,1-2H3
InchiKey: IYBYEHHNRLOTHL-UHFFFAOYSA-N
Formula: C12H21F3O2
SMILES: CCCCCCCCC(C)OC(=O)C(F)(F)F
Mol. weight [g/mol]: 254.29

Physical Properties

Property code	Value	Unit	Source
gf	-767.79	kJ/mol	Joback Method
hf	-1138.17	kJ/mol	Joback Method
hfus	27.93	kJ/mol	Joback Method
hvap	47.33	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	4.231		Crippen Method
mcvol	192.690	ml/mol	McGowan Method
pc	1690.72	kPa	Joback Method
rinpol	1192.20		NIST Webbook
rinpol	1192.20		NIST Webbook
tb	544.39	K	Joback Method
tc	704.83	K	Joback Method
tf	286.35	K	Joback Method
vc	0.768	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.72	J/mol×K	544.39	Joback Method
cpg	506.64	J/mol×K	571.13	Joback Method
cpg	520.92	J/mol×K	597.87	Joback Method
cpg	534.56	J/mol×K	624.61	Joback Method
cpg	547.58	J/mol×K	651.35	Joback Method
cpg	560.01	J/mol×K	678.09	Joback Method
cpg	571.85	J/mol×K	704.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352328&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume