trans-2-Dodecen-1-ol, trifluoroacetate

Inchi: InChI=1S/C14H23F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-19-13(18)14(15,16)17/h10-11H,2-9
InchiKey: WMJRRZIEUNTJJE-ZHACJKMWSA-N
Formula: C14H23F3O2
SMILES: CCCCCCCCCC=CCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 280.33

Physical Properties

Property code	Value	Unit	Source
gf	-668.29	kJ/mol	Joback Method
hf	-1056.95	kJ/mol	Joback Method
hfus	36.83	kJ/mol	Joback Method
hvap	52.12	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.789		Crippen Method
mcvol	216.570	ml/mol	McGowan Method
pc	1502.31	kPa	Joback Method
rinpol	1436.70		NIST Webbook
rinpol	1436.70		NIST Webbook
tb	594.75	K	Joback Method
tc	757.42	K	Joback Method
tf	318.81	K	Joback Method
vc	0.867	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.43	J/mol×K	594.75	Joback Method
cpg	589.78	J/mol×K	621.86	Joback Method
cpg	604.40	J/mol×K	648.97	Joback Method
cpg	618.34	J/mol×K	676.09	Joback Method
cpg	631.61	J/mol×K	703.20	Joback Method
cpg	644.25	J/mol×K	730.31	Joback Method
cpg	656.28	J/mol×K	757.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352262&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