

trans-2-Decen-1-ol, trifluoroacetate

Inchi: InChI=1S/C12H19F3O2/c1-2-3-4-5-6-7-8-9-10-17-11(16)12(13,14)15/h8-9H,2-7,10H2,1H
InchiKey: WBRGXAXCDNMVNG-CMDGGGOBGSA-N
Formula: C12H19F3O2
SMILES: CCCCCC=CCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 252.27

Physical Properties

Property code	Value	Unit	Source
gf	-685.13	kJ/mol	Joback Method
hf	-1015.67	kJ/mol	Joback Method
hfus	31.65	kJ/mol	Joback Method
hvap	47.67	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	4.009		Crippen Method
mcvol	188.390	ml/mol	McGowan Method
pc	1753.60	kPa	Joback Method
rinpola	1253.50		NIST Webbook
rinpola	1253.50		NIST Webbook
tb	548.99	K	Joback Method
tc	712.64	K	Joback Method
tf	296.27	K	Joback Method
vc	0.754	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.19	J/molxK	548.99	Joback Method
cpg	487.45	J/molxK	576.26	Joback Method
cpg	501.03	J/molxK	603.54	Joback Method
cpg	513.97	J/molxK	630.81	Joback Method
cpg	526.28	J/molxK	658.09	Joback Method
cpg	538.00	J/molxK	685.36	Joback Method
cpg	549.14	J/molxK	712.64	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U352670&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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