

Acetic acid, trifluoro-, dodecyl ester

Other names:	Dodecyl trifluoroacetate Trifluoroacetic acid, dodecyl ester
Inchi:	InChI=1S/C14H25F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-19-13(18)14(15,16)17/h2-12H2,1H1
InchiKey:	RXTXOEGLTCFHGU-UHFFFAOYSA-N
Formula:	C14H25F3O2
SMILES:	CCCCCCCCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]:	282.34
CAS:	6222-00-0

Physical Properties

Property code	Value	Unit	Source
gf	-748.51	kJ/mol	Joback Method
hf	-1174.17	kJ/mol	Joback Method
hfus	36.63	kJ/mol	Joback Method
hvap	52.17	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	5.013		Crippen Method
mcvol	220.870	ml/mol	McGowan Method
pc	1443.54	kPa	Joback Method
rinpol	1432.00		NIST Webbook
rinpol	1439.70		NIST Webbook
rinpol	1418.00		NIST Webbook
rinpol	1421.00		NIST Webbook
ripol	1555.00		NIST Webbook
tb	590.59	K	Joback Method
tc	748.20	K	Joback Method
tf	323.89	K	Joback Method
vc	0.886	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.85	J/mol×K	590.59	Joback Method
cpg	609.61	J/mol×K	616.86	Joback Method

cpg	624.68	J/mol×K	643.13	Joback Method
cpg	639.09	J/mol×K	669.39	Joback Method
cpg	652.85	J/mol×K	695.66	Joback Method
cpg	665.99	J/mol×K	721.93	Joback Method
cpg	678.53	J/mol×K	748.20	Joback Method

Sources

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=C6222000&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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