Tetradecyl trifluoroacetate

Inchi: InChI=1S/C16H29F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-21-15(20)16(17,18)19/h2-14
InchiKey: UVIFJLAXCAKUFR-UHFFFAOYSA-N
Formula: C16H29F3O2
SMILES: CCCCCCCCCCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 310.40
CAS: 6222-02-2

Physical Properties

Property code	Value	Unit	Source
gf	-731.67	kJ/mol	Joback Method
hf	-1215.45	kJ/mol	Joback Method
hfus	41.81	kJ/mol	Joback Method
hvap	56.62	kJ/mol	Joback Method
log10ws	-6.05		Crippen Method
logp	5.793		Crippen Method
mcvol	249.050	ml/mol	McGowan Method
pc	1253.92	kPa	Joback Method
rinpol	1630.10		NIST Webbook
rinpol	1620.00		NIST Webbook
rinpol	1617.40		NIST Webbook
rinpol	1620.00		NIST Webbook
rinpol	1630.10		NIST Webbook
rinpol	1617.40		NIST Webbook
tb	636.35	K	Joback Method
tc	794.99	K	Joback Method
tf	346.43	K	Joback Method
vc	0.999	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.02	J/mol×K	636.35	Joback Method
cpg	718.77	J/mol×K	662.79	Joback Method
cpg	734.79	J/mol×K	689.23	Joback Method

cpg	750.07	J/mol×K	715.67	Joback Method
cpg	764.67	J/mol×K	742.11	Joback Method
cpg	778.58	J/mol×K	768.55	Joback Method
cpg	791.84	J/mol×K	794.99	Joback Method

Sources

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=C6222022&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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