Docosyl trifluoroacetate

Other names: Docosyl 2,2,2-trifluoroacetate
1-Docosanol, trifluoroacetate
Inchi: InChI=1S/C24H45F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-29
InchiKey: CNPFIRPKOQTKAO-UHFFFAOYSA-N
Formula: C24H45F3O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 422.61

Physical Properties

Property code	Value	Unit	Source
gf	-664.31	kJ/mol	Joback Method
hf	-1380.57	kJ/mol	Joback Method
hfus	62.53	kJ/mol	Joback Method
hvap	74.43	kJ/mol	Joback Method
log10ws	-9.39		Crippen Method
logp	8.914		Crippen Method
mcvol	361.770	ml/mol	McGowan Method
pc	775.05	kPa	Joback Method
rinpol	2393.70		NIST Webbook
rinpol	2393.70		NIST Webbook
tb	819.39	K	Joback Method
tc	1003.83	K	Joback Method
tf	436.59	K	Joback Method
vc	1.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1179.16	J/mol×K	819.39	Joback Method
cpg	1200.28	J/mol×K	850.13	Joback Method
cpg	1220.25	J/mol×K	880.87	Joback Method
cpg	1239.12	J/mol×K	911.61	Joback Method
cpg	1256.94	J/mol×K	942.35	Joback Method
cpg	1273.76	J/mol×K	973.09	Joback Method

cpg	1289.64	J/mol×K	1003.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U351755&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