

«beta»-Tocopherol, O-heptafluorobutyryl-

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C32H47F7O3/c1-20(2)11-8-12-21(3)13-9-14-22(4)15-10-17-29(7)18-16-25-24(6)23

NCOOQQVRNBXILQ-UHFFFAOYSA-N

C32H47F7O3

Cc1cc(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)c(C)c2c1OC(C)(CCCC(C)CCCC(C)CCCC(C)C)C2

612.70

Physical Properties

Property code	Value	Unit	Source
gf	-1346.90	kJ/mol	Joback Method
hf	-2222.94	kJ/mol	Joback Method
hfus	60.37	kJ/mol	Joback Method
hvap	93.58	kJ/mol	Joback Method
log10ws	-12.18		Crippen Method
logp	10.565		Crippen Method
mcvol	452.820	ml/mol	McGowan Method
pc	620.03	kPa	Joback Method
rinpol	2843.00		NIST Webbook
rinpol	2843.00		NIST Webbook
tb	1076.53	K	Joback Method
tc	1334.91	K	Joback Method
tf	630.34	K	Joback Method
vc	1.786	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1664.76	J/mol×K	1076.53	Joback Method
cpg	1695.11	J/mol×K	1119.59	Joback Method
cpg	1726.02	J/mol×K	1162.66	Joback Method
cpg	1757.90	J/mol×K	1205.72	Joback Method
cpg	1791.15	J/mol×K	1248.78	Joback Method
cpg	1826.17	J/mol×K	1291.85	Joback Method
cpg	1863.37	J/mol×K	1334.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374741&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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