«alpha»-Terpineol, «beta»-D-glucopyranoside, TFA

Other names: «alpha»-terpineyl «beta»-D-glucopyranoside, TFA
«alpha»-Terpineol, B-D-Glu, TFA

Inchi: InChI=1S/C24H24F12O10/c1-9-4-6-10(7-5-9)20(2,3)46-15-14(45-19(40)24(34,35)36)13(

InchiKey: DMNHAEJEIAAJSG-UHFFFAOYSA-N

Formula: C24H24F12O10

SMILES: CC1=CCC(C(C)(C)OC2OC(COC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C

Mol. weight [g/mol]: 700.42

Physical Properties

Property code	Value	Unit	Source
gf	-3260.73	kJ/mol	Joback Method
hf	-4105.59	kJ/mol	Joback Method
hfus	66.91	kJ/mol	Joback Method
hvap	96.85	kJ/mol	Joback Method
log10ws	-6.71		Crippen Method
logp	4.781		Crippen Method
mcvol	385.740	ml/mol	McGowan Method
pc	811.68	kPa	Joback Method
rinpol	1936.00		NIST Webbook
rinpol	1946.00		NIST Webbook
rinpol	1936.00		NIST Webbook
rinpol	1918.00		NIST Webbook
rinpol	1918.00		NIST Webbook
rinpol	1946.00		NIST Webbook
rinpol	1936.00		NIST Webbook
tb	1102.70	K	Joback Method
tc	1372.98	K	Joback Method
tf	727.94	K	Joback Method
vc	1.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1407.62	J/mol×K	1102.70	Joback Method

cpg	1415.08	J/mol×K	1147.75	Joback Method
cpg	1419.98	J/mol×K	1192.79	Joback Method
cpg	1422.46	J/mol×K	1237.84	Joback Method
cpg	1422.67	J/mol×K	1282.89	Joback Method
cpg	1420.75	J/mol×K	1327.94	Joback Method
cpg	1416.86	J/mol×K	1372.98	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=R70656&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