Fumaric acid, bis-(2,2,2-trifluoroethyl)ester-

Inchi: InChI=1S/C8H6F6O4/c9-7(10,11)3-17-5(15)1-2-6(16)18-4-8(12,13)14/h1-2H,3-4H2/b2-1
InchiKey: KZTDZFZLDVZRCF-OWOJBTEDSA-N
Formula: C8H6F6O4
SMILES: O=C(C=CC(=O)OCC(F)(F)F)OCC(F)(F)F
Mol. weight [g/mol]: 280.12
CAS: 352-28-3

Physical Properties

Property code	Value	Unit	Source
gf	-1534.32	kJ/mol	Joback Method
hf	-1774.99	kJ/mol	Joback Method
hfus	25.90	kJ/mol	Joback Method
hvap	44.18	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	1.754		Crippen Method
mcvol	144.780	ml/mol	McGowan Method
pc	2324.78	kPa	Joback Method
tb	528.34	K	Joback Method
tc	691.34	K	Joback Method
tf	327.54	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.34	J/mol×K	528.34	Joback Method
cpg	369.82	J/mol×K	555.51	Joback Method
cpg	378.74	J/mol×K	582.67	Joback Method
cpg	387.12	J/mol×K	609.84	Joback Method
cpg	395.00	J/mol×K	637.01	Joback Method
cpg	402.38	J/mol×K	664.17	Joback Method
cpg	409.30	J/mol×K	691.34	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=C352283&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume