Diethyl perfluoroglutarate

Other names:	Pentanedioic acid, hexafluoro-, diethyl ester
	Diethyl hexafluoroglutarate
	Hexafluroglutaric acid diethyl ester
	Glutaric acid, hexafluoro-, diethyl ester
	Diethylester kyseliny hexafluorglutarove
	Hexafluoroglutaric acid diethyl ester
	Hexafluoropentanedioic acid diethyl ester
	Diethyl 2,2,3,3,4,4-hexafluoropentanedioate
	NSC 63360
	Pentanedioic acid, 2,2,3,3,4,4-hexafluoro-, 1,5-diethyl ester
Inchi:	InChI=1S/C9H10F6O4/c1-3-18-5(16)7(10,11)9(14,15)8(12,13)6(17)19-4-2/h3-4H2,1-2H3
InchiKey:	MSDPXVBLFJODJO-UHFFFAOYSA-N
Formula:	C9H10F6O4
SMILES:	CCOC(=O)C(F)(F)C(F)(F)C(F)(F)C(=O)OCC
Mol. weight [g/mol]:	296.16
CAS:	424-40-8

Physical Properties

Property code	Value	Unit	Source
gf	-1603.28	kJ/mol	Joback Method
hf	-1921.60	kJ/mol	Joback Method
hfus	20.88	kJ/mol	Joback Method
hvap	45.15	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	2.019		Crippen Method
mcvol	163.170	ml/mol	McGowan Method
pc	2060.49	kPa	Joback Method
tb	543.83	K	Joback Method
tc	707.82	K	Joback Method
tf	346.31	K	Joback Method
vc	0.662	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.58	J/mol×K	543.83	Joback Method
cpg	438.86	J/mol×K	571.16	Joback Method
cpg	449.48	J/mol×K	598.49	Joback Method
cpg	459.46	J/mol×K	625.82	Joback Method
cpg	468.82	J/mol×K	653.16	Joback Method
cpg	477.59	J/mol×K	680.49	Joback Method
cpg	485.80	J/mol×K	707.82	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	350.50 ± 2.50	K	0.40	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C424408&Units=SI

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
tbrp: Boiling point at reduced pressure

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume