Fumaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl pentyl ester

Inchi: InChI=1S/C14H16F8O4/c1-2-3-4-7-25-9(23)5-6-10(24)26-8-12(17,18)14(21,22)13(19,20)

InchiKey: RRRZLVOBFDUMRO-AATRIKPKSA-N

Formula: C14H16F8O4

SMILES: CCCCCOC(=O)C=CC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 400.26

Physical Properties

Property code	Value	Unit	Source
gf	-1873.02	kJ/mol	Joback Method
hf	-2305.08	kJ/mol	Joback Method
hfus	36.67	kJ/mol	Joback Method
hvap	54.22	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.990		Crippen Method
mcvol	232.860	ml/mol	McGowan Method
pc	1358.63	kPa	Joback Method
rinpol	1578.00		NIST Webbook
rinpol	1578.00		NIST Webbook
tb	660.49	K	Joback Method
tc	821.51	K	Joback Method
tf	383.76	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.38	J/mol×K	660.49	Joback Method
cpg	685.05	J/mol×K	687.33	Joback Method
cpg	696.98	J/mol×K	714.16	Joback Method
cpg	708.19	J/mol×K	741.00	Joback Method
cpg	718.73	J/mol×K	767.84	Joback Method
cpg	728.63	J/mol×K	794.68	Joback Method
cpg	737.94	J/mol×K	821.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348780&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

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