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

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

InchiKey: IVRZADLFRIWRDA-ONEGZZNKSA-N

Formula: C14H16F8O4

SMILES: CC(C)CCOC(=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	-1875.46	kJ/mol	Joback Method
hf	-2310.36	kJ/mol	Joback Method
hfus	33.14	kJ/mol	Joback Method
hvap	53.83	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.846		Crippen Method
mcvol	232.860	ml/mol	McGowan Method
pc	1366.68	kPa	Joback Method
rinpol	1548.00		NIST Webbook
rinpol	1548.00		NIST Webbook
tb	660.05	K	Joback Method
tc	822.71	K	Joback Method
tf	368.76	K	Joback Method
vc	0.947	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.85	J/mol×K	660.05	Joback Method
cpg	685.69	J/mol×K	687.16	Joback Method
cpg	697.75	J/mol×K	714.27	Joback Method
cpg	709.09	J/mol×K	741.38	Joback Method
cpg	719.72	J/mol×K	768.49	Joback Method
cpg	729.71	J/mol×K	795.60	Joback Method
cpg	739.09	J/mol×K	822.71	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=U405547&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

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