Fumaric acid, 2-(2-methoxyethyl)hexyl 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C18H24F8O5/c1-3-4-5-12(8-9-29-2)10-30-13(27)6-7-14(28)31-11-16(21,22)18

InchiKey: GYNNJQIEDIQPAY-VOTSOKGWSA-N

Formula: C18H24F8O5

SMILES: CCCCC(CCOC)COC(=O)C=CC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 472.37

Physical Properties

Property code	Value	Unit	Source
gf	-1946.78	kJ/mol	Joback Method
hf	-2525.14	kJ/mol	Joback Method
hfus	44.69	kJ/mol	Joback Method
hvap	65.14	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.643		Crippen Method
mcvol	295.090	ml/mol	McGowan Method
pc	1036.57	kPa	Joback Method
rinpol	1961.00		NIST Webbook
tb	773.99	K	Joback Method
tc	948.50	K	Joback Method
tf	436.07	K	Joback Method
vc	1.188	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	921.67	J/mol×K	773.99	Joback Method
cpg	936.15	J/mol×K	803.07	Joback Method
cpg	949.74	J/mol×K	832.16	Joback Method
cpg	962.47	J/mol×K	861.24	Joback Method
cpg	974.40	J/mol×K	890.33	Joback Method
cpg	985.57	J/mol×K	919.41	Joback Method
cpg	996.03	J/mol×K	948.50	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=U405892&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