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

Inchi: InChI=1S/C20H28F8O5/c1-3-4-6-14(10-12-31-2)7-5-11-32-15(29)8-9-16(30)33-13-18(23

InchiKey: DZLWHTMILUZOQP-CMDGGOBGSA-N

Formula: C20H28F8O5

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

Mol. weight [g/mol]: 500.42

Physical Properties

Property code	Value	Unit	Source
gf	-1929.94	kJ/mol	Joback Method
hf	-2566.42	kJ/mol	Joback Method
hfus	49.87	kJ/mol	Joback Method
hvap	69.59	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	5.423		Crippen Method
mcvol	323.270	ml/mol	McGowan Method
pc	919.39	kPa	Joback Method
rinpol	2072.00		NIST Webbook
tb	819.75	K	Joback Method
tc	1003.72	K	Joback Method
tf	458.61	K	Joback Method
vc	1.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1037.98	J/mol×K	819.75	Joback Method
cpg	1053.54	J/mol×K	850.41	Joback Method
cpg	1068.09	J/mol×K	881.07	Joback Method
cpg	1081.70	J/mol×K	911.73	Joback Method
cpg	1094.42	J/mol×K	942.40	Joback Method
cpg	1106.32	J/mol×K	973.06	Joback Method
cpg	1117.46	J/mol×K	1003.72	Joback Method

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=U405910&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume