

Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl undec-2-enyl ester

Inchi:	InChI=1S/C21H30F8O4/c1-2-3-4-5-6-7-8-9-10-14-32-16(30)12-11-13-17(31)33-15-19(24
InchiKey:	DZARZFOLDSMPJA-MDZDMXLPSA-N
Formula:	C21H30F8O4
SMILES:	CCCCCCCC=CCOC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F
Mol. weight [g/mol]:	498.45

Physical Properties

Property code	Value	Unit	Source
gf	-1814.08	kJ/mol	Joback Method
hf	-2449.56	kJ/mol	Joback Method
hfus	54.80	kJ/mol	Joback Method
hvap	69.80	kJ/mol	Joback Method
log10ws	-7.45		Crippen Method
logp	6.721		Crippen Method
mvol	331.490	ml/mol	McGowan Method
pc	872.74	kPa	Joback Method
rinpol	2186.00		NIST Webbook
rinpol	2186.00		NIST Webbook
tb	820.65	K	Joback Method
tc	1005.15	K	Joback Method
tf	462.65	K	Joback Method
vc	1.345	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1066.60	J/mol×K	820.65	Joback Method
cpg	1082.85	J/mol×K	851.40	Joback Method
cpg	1098.10	J/mol×K	882.15	Joback Method
cpg	1112.44	J/mol×K	912.90	Joback Method
cpg	1125.93	J/mol×K	943.65	Joback Method
cpg	1138.65	J/mol×K	974.40	Joback Method
cpg	1150.67	J/mol×K	1005.15	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U394012&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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