Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl oct-3-en-2-yl ester

Inchi: InChI=1S/C18H24F8O4/c1-3-4-5-6-8-12(2)30-14(28)10-7-9-13(27)29-11-16(21,22)18(25

InchiKey: AXBFZWYUIZCEAR-SOFGYWHQSA-N

Formula: C18H24F8O4

SMILES: CCCCC=CC(C)OC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 456.37

Physical Properties

Property code	Value	Unit	Source
gf	-1841.78	kJ/mol	Joback Method
hf	-2392.92	kJ/mol	Joback Method
hfus	43.50	kJ/mol	Joback Method
hvap	62.73	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	5.549		Crippen Method
mcvol	289.220	ml/mol	McGowan Method
pc	1048.01	kPa	Joback Method
rinpol	1819.00		NIST Webbook
rinpol	1819.00		NIST Webbook
tb	751.57	K	Joback Method
tc	922.41	K	Joback Method
tf	413.84	K	Joback Method
vc	1.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	892.42	J/mol×K	751.57	Joback Method
cpg	907.03	J/mol×K	780.04	Joback Method
cpg	920.76	J/mol×K	808.52	Joback Method
cpg	933.68	J/mol×K	836.99	Joback Method
cpg	945.83	J/mol×K	865.46	Joback Method
cpg	957.27	J/mol×K	893.94	Joback Method
cpg	968.04	J/mol×K	922.41	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=U393983&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