Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl cis-hex-3-enyl ester

Inchi: InChI=1S/C16H20F8O4/c1-2-3-4-5-9-27-11(25)7-6-8-12(26)28-10-14(19,20)16(23,24)15

InchiKey: BUZFIMIZKLPIRZ-ARJAWSKDSA-N

Formula: C16H20F8O4

SMILES: CCC=CCCOC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 428.31

Physical Properties

Property code	Value	Unit	Source
gf	-1856.18	kJ/mol	Joback Method
hf	-2346.36	kJ/mol	Joback Method
hfus	41.85	kJ/mol	Joback Method
hvap	58.67	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.770		Crippen Method
mcvol	261.040	ml/mol	McGowan Method
pc	1184.97	kPa	Joback Method
rinpol	1723.00		NIST Webbook
rinpol	1723.00		NIST Webbook
tb	706.25	K	Joback Method
tc	870.71	K	Joback Method
tf	406.30	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	780.02	J/mol×K	706.25	Joback Method
cpg	793.60	J/mol×K	733.66	Joback Method
cpg	806.39	J/mol×K	761.07	Joback Method
cpg	818.42	J/mol×K	788.48	Joback Method
cpg	829.74	J/mol×K	815.89	Joback Method
cpg	840.39	J/mol×K	843.30	Joback Method
cpg	850.43	J/mol×K	870.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U394022&Units=SI
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

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