Glutaric acid, hexa-1,5-dien-3-yl 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C16H18F8O4/c1-3-6-10(4-2)28-12(26)8-5-7-11(25)27-9-14(19,20)16(23,24)15

InchiKey: OPLURIHZQSQRNT-UHFFFAOYSA-N

Formula: C16H18F8O4

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

Mol. weight [g/mol]: 426.30

Physical Properties

Property code	Value	Unit	Source
gf	-1763.16	kJ/mol	Joback Method
hf	-2218.00	kJ/mol	Joback Method
hfus	35.56	kJ/mol	Joback Method
hvap	56.98	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.545		Crippen Method
mcvol	256.740	ml/mol	McGowan Method
pc	1218.29	kPa	Joback Method
rinpol	1613.00		NIST Webbook
rinpol	1613.00		NIST Webbook
tb	695.01	K	Joback Method
tc	859.09	K	Joback Method
tf	392.86	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.53	J/mol×K	695.01	Joback Method
cpg	768.75	J/mol×K	722.36	Joback Method
cpg	781.16	J/mol×K	749.70	Joback Method
cpg	792.82	J/mol×K	777.05	Joback Method
cpg	803.76	J/mol×K	804.40	Joback Method
cpg	814.02	J/mol×K	831.74	Joback Method
cpg	823.65	J/mol×K	859.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405273&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

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