Glutaric acid, di(2,2,3,3,4,4,5,5-octafluoropentyl) ester

Inchi: InChI=1S/C15H12F16O4/c16-8(17)12(24,25)14(28,29)10(20,21)4-34-6(32)2-1-3-7(33)35
InchiKey: XCUIUACVMRRNFF-UHFFFAOYSA-N
Formula: C15H12F16O4
SMILES: O=C(CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)F)OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)F
Mol. weight [g/mol]: 560.23

Physical Properties

Property code	Value	Unit	Source
gf	-3497.22	kJ/mol	Joback Method
hf	-4043.35	kJ/mol	Joback Method
hfus	37.93	kJ/mol	Joback Method
hvap	45.67	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	5.585		Crippen Method
mcvol	265.410	ml/mol	McGowan Method
pc	1003.98	kPa	Joback Method
rinpol	1556.00		NIST Webbook
rinpol	1556.00		NIST Webbook
tb	663.24	K	Joback Method
tc	812.76	K	Joback Method
tf	397.09	K	Joback Method
vc	1.133	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.77	J/mol×K	663.24	Joback Method
cpg	832.03	J/mol×K	688.16	Joback Method
cpg	843.45	J/mol×K	713.08	Joback Method
cpg	854.09	J/mol×K	738.00	Joback Method
cpg	863.98	J/mol×K	762.92	Joback Method
cpg	873.19	J/mol×K	787.84	Joback Method
cpg	881.77	J/mol×K	812.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359694&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