Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl neopentyl ester

Inchi: InChI=1S/C15H20F8O4/c1-12(2,3)7-26-9(24)5-4-6-10(25)27-8-13(18,19)15(22,23)14(20,

InchiKey: YXAXICLINGOTIC-UHFFFAOYSA-N

Formula: C15H20F8O4

SMILES: CC(C)(C)COC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 416.30

Physical Properties

Property code	Value	Unit	Source
gf	-1941.98	kJ/mol	Joback Method
hf	-2451.69	kJ/mol	Joback Method
hfus	31.64	kJ/mol	Joback Method
hvap	55.19	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.460		Crippen Method
mcvol	251.250	ml/mol	McGowan Method
pc	1238.09	kPa	Joback Method
rinpol	1543.00		NIST Webbook
rinpol	1543.00		NIST Webbook
tb	675.98	K	Joback Method
tc	838.72	K	Joback Method
tf	402.53	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.53	J/mol×K	675.98	Joback Method
cpg	764.42	J/mol×K	703.10	Joback Method
cpg	777.47	J/mol×K	730.23	Joback Method
cpg	789.72	J/mol×K	757.35	Joback Method
cpg	801.23	J/mol×K	784.47	Joback Method
cpg	812.03	J/mol×K	811.59	Joback Method
cpg	822.16	J/mol×K	838.72	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=U391605&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