Glutaric acid, 2,2,3,3,4,4,4-heptafluorobutyl hexyl ester

Inchi: InChI=1S/C15H21F7O4/c1-2-3-4-5-9-25-11(23)7-6-8-12(24)26-10-13(16,17)14(18,19)15

InchiKey: OQUOBKHCBWZFFU-UHFFFAOYSA-N

Formula: C15H21F7O4

SMILES: CCCCCCOC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 398.31

Physical Properties

Property code	Value	Unit	Source
gf	-1747.57	kJ/mol	Joback Method
hf	-2241.55	kJ/mol	Joback Method
hfus	39.50	kJ/mol	Joback Method
hvap	57.69	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.656		Crippen Method
mcvol	249.480	ml/mol	McGowan Method
pc	1253.92	kPa	Joback Method
rinpol	1736.00		NIST Webbook
tb	680.38	K	Joback Method
tc	841.49	K	Joback Method
tf	414.52	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.59	J/mol×K	680.38	Joback Method
cpg	753.50	J/mol×K	707.23	Joback Method
cpg	766.63	J/mol×K	734.08	Joback Method
cpg	779.03	J/mol×K	760.93	Joback Method
cpg	790.71	J/mol×K	787.79	Joback Method
cpg	801.72	J/mol×K	814.64	Joback Method
cpg	812.09	J/mol×K	841.49	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=U377551&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