Glutaric acid, 2,2,3,3,4,4,4-heptafluorobutyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C16H23F7O4/c1-4-6-11(10(2)3)27-13(25)8-5-7-12(24)26-9-14(17,18)15(19,20)

InchiKey: LKUYMUWIJZSHJM-UHFFFAOYSA-N

Formula: C16H23F7O4

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

Mol. weight [g/mol]: 412.34

Physical Properties

Property code	Value	Unit	Source
gf	-1744.03	kJ/mol	Joback Method
hf	-2272.75	kJ/mol	Joback Method
hfus	35.04	kJ/mol	Joback Method
hvap	59.14	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.901		Crippen Method
mcvol	263.570	ml/mol	McGowan Method
pc	1185.79	kPa	Joback Method
rinpol	1696.00		NIST Webbook
rinpol	1696.00		NIST Webbook
tb	702.38	K	Joback Method
tc	867.88	K	Joback Method
tf	395.79	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.60	J/mol×K	702.38	Joback Method
cpg	810.23	J/mol×K	729.96	Joback Method
cpg	824.01	J/mol×K	757.55	Joback Method
cpg	836.99	J/mol×K	785.13	Joback Method
cpg	849.20	J/mol×K	812.71	Joback Method
cpg	860.68	J/mol×K	840.30	Joback Method
cpg	871.48	J/mol×K	867.88	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377550&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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