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

Inchi: InChI=1S/C27H45F7O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-37-23(35)19-18

InchiKey: XKMBODQKCJBHJE-UHFFFAOYSA-N

Formula: C27H45F7O4

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

Mol. weight [g/mol]: 566.63

Physical Properties

Property code	Value	Unit	Source
gf	-1646.53	kJ/mol	Joback Method
hf	-2489.23	kJ/mol	Joback Method
hfus	70.58	kJ/mol	Joback Method
hvap	84.40	kJ/mol	Joback Method
log10ws	-10.14		Crippen Method
logp	9.338		Crippen Method
mcvol	418.560	ml/mol	McGowan Method
pc	632.57	kPa	Joback Method
rinpol	2981.00		NIST Webbook
rinpol	2981.00		NIST Webbook
tb	954.94	K	Joback Method
tc	1196.16	K	Joback Method
tf	549.76	K	Joback Method
vc	1.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1456.42	J/mol×K	954.94	Joback Method
cpg	1478.65	J/mol×K	995.14	Joback Method
cpg	1499.23	J/mol×K	1035.35	Joback Method
cpg	1518.33	J/mol×K	1075.55	Joback Method
cpg	1536.13	J/mol×K	1115.75	Joback Method
cpg	1552.78	J/mol×K	1155.96	Joback Method
cpg	1568.47	J/mol×K	1196.16	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377563&Units=SI

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

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