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

Inchi: InChI=1S/C17H25F7O4/c1-2-3-4-5-6-7-11-27-13(25)9-8-10-14(26)28-12-15(18,19)16(20
InchiKey: SDFLHZQHOPCPQH-UHFFFAOYSA-N
Formula: C17H25F7O4
SMILES: CCCCCCCCOC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 426.37

Physical Properties

Property code	Value	Unit	Source
gf	-1730.73	kJ/mol	Joback Method
hf	-2282.83	kJ/mol	Joback Method
hfus	44.68	kJ/mol	Joback Method
hvap	62.14	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	5.437		Crippen Method
mcvol	277.660	ml/mol	McGowan Method
pc	1099.35	kPa	Joback Method
rinpol	1942.00		NIST Webbook
rinpol	1942.00		NIST Webbook
tb	726.14	K	Joback Method
tc	892.08	K	Joback Method
tf	437.06	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.72	J/mol×K	726.14	Joback Method
cpg	865.58	J/mol×K	753.80	Joback Method
cpg	879.59	J/mol×K	781.45	Joback Method
cpg	892.80	J/mol×K	809.11	Joback Method
cpg	905.24	J/mol×K	836.77	Joback Method
cpg	916.97	J/mol×K	864.42	Joback Method
cpg	928.00	J/mol×K	892.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377553&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