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

Inchi: InChI=1S/C29H49F7O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23-39-25(37

InchiKey: CRKMZXNTODIMTR-UHFFFAOYSA-N

Formula: C29H49F7O4

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

Mol. weight [g/mol]: 594.69

Physical Properties

Property code	Value	Unit	Source
gf	-1629.69	kJ/mol	Joback Method
hf	-2530.51	kJ/mol	Joback Method
hfus	75.76	kJ/mol	Joback Method
hvap	88.85	kJ/mol	Joback Method
log10ws	-10.98		Crippen Method
logp	10.118		Crippen Method
mcvol	446.740	ml/mol	McGowan Method
pc	575.63	kPa	Joback Method
rinpol	3184.00		NIST Webbook
rinpol	3184.00		NIST Webbook
tb	1000.70	K	Joback Method
tc	1272.13	K	Joback Method
tf	572.30	K	Joback Method
vc	1.800	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1584.80	J/mol×K	1000.70	Joback Method
cpg	1609.52	J/mol×K	1045.94	Joback Method
cpg	1632.28	J/mol×K	1091.18	Joback Method
cpg	1653.34	J/mol×K	1136.41	Joback Method
cpg	1672.95	J/mol×K	1181.65	Joback Method
cpg	1691.39	J/mol×K	1226.89	Joback Method
cpg	1708.89	J/mol×K	1272.13	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=U377564&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