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

Inchi: InChI=1S/C26H43F7O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-36-22(34)18-17-19

InchiKey: AXUGLVQHJSEJIV-UHFFFAOYSA-N

Formula: C26H43F7O4

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

Mol. weight [g/mol]: 552.61

Physical Properties

Property code	Value	Unit	Source
gf	-1654.95	kJ/mol	Joback Method
hf	-2468.59	kJ/mol	Joback Method
hfus	67.99	kJ/mol	Joback Method
hvap	82.17	kJ/mol	Joback Method
log10ws	-9.72		Crippen Method
logp	8.947		Crippen Method
mcvol	404.470	ml/mol	McGowan Method
pc	664.26	kPa	Joback Method
rinpol	2879.00		NIST Webbook
rinpol	2879.00		NIST Webbook
tb	932.06	K	Joback Method
tc	1160.55	K	Joback Method
tf	538.49	K	Joback Method
vc	1.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1392.96	J/mol×K	932.06	Joback Method
cpg	1414.11	J/mol×K	970.14	Joback Method
cpg	1433.75	J/mol×K	1008.22	Joback Method
cpg	1452.01	J/mol×K	1046.31	Joback Method
cpg	1469.04	J/mol×K	1084.39	Joback Method
cpg	1484.97	J/mol×K	1122.47	Joback Method
cpg	1499.95	J/mol×K	1160.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377562&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