

Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C14H12F14O4/c15-8(13(24,25)26)10(18,19)4-31-6(29)2-1-3-7(30)32-5-11(20,21)33

InchiKey: LXVKZIXJUCXKKW-UHFFFAOYSA-N

Formula: C14H12F14O4

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

Mol. weight [g/mol]: 510.22

Physical Properties

Property code	Value	Unit	Source
gf	-3118.86	kJ/mol	Joback Method
hf	-3621.74	kJ/mol	Joback Method
hfus	36.59	kJ/mol	Joback Method
hvap	46.38	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	4.950		Crippen Method
mvol	247.780	ml/mol	McGowan Method
pc	1119.30	kPa	Joback Method
rinpol	1413.00		NIST Webbook
rinpol	1413.00		NIST Webbook
tb	645.05	K	Joback Method
tc	792.84	K	Joback Method
tf	382.22	K	Joback Method
vc	1.052	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	748.07	J/molxK	645.05	Joback Method
cpg	760.17	J/molxK	669.68	Joback Method
cpg	771.50	J/molxK	694.31	Joback Method
cpg	782.08	J/molxK	718.95	Joback Method
cpg	791.98	J/molxK	743.58	Joback Method
cpg	801.22	J/molxK	768.21	Joback Method
cpg	809.85	J/molxK	792.84	Joback Method

Sources

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=U393683&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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