

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

Inchi:	InChI=1S/C21H33F7O4/c1-2-3-4-5-6-7-8-9-10-11-15-31-17(29)13-12-14-18(30)32-16-19
InchiKey:	YVJMOQPGHJMISW-UHFFFAOYSA-N
Formula:	C21H33F7O4
SMILES:	CCCCCCCCCCCCOC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	482.47

Physical Properties

Property code	Value	Unit	Source
gf	-1697.05	kJ/mol	Joback Method
hf	-2365.39	kJ/mol	Joback Method
hfus	55.04	kJ/mol	Joback Method
hvap	71.05	kJ/mol	Joback Method
log10ws	-7.63		Crippen Method
logp	6.997		Crippen Method
mcvol	334.020	ml/mol	McGowan Method
pc	865.05	kPa	Joback Method
rinsol	2358.00		NIST Webbook
tb	817.66	K	Joback Method
tc	1001.67	K	Joback Method
tf	482.14	K	Joback Method
vc	1.353	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1084.34	J/molxK	817.66	Joback Method
cpg	1101.42	J/molxK	848.33	Joback Method
cpg	1117.45	J/molxK	879.00	Joback Method
cpg	1132.49	J/molxK	909.66	Joback Method
cpg	1146.61	J/molxK	940.33	Joback Method
cpg	1159.87	J/molxK	971.00	Joback Method
cpg	1172.33	J/molxK	1001.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377557&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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