

Glutaric acid, 2-(adamant-1-yl)ethyl 2-ethylhexyl ester

Inchi:	InChI=1S/C25H42O4/c1-3-5-7-19(4-2)18-29-24(27)9-6-8-23(26)28-11-10-25-15-20-12-21
InchiKey:	IBPPMQXLKKRRQR-UHFFFAOYSA-N
Formula:	C25H42O4
SMILES:	CCCCC(CC)COC(=O)CCCC(=O)OCCC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	406.60

Physical Properties

Property code	Value	Unit	Source
gf	-153.71	kJ/mol	Joback Method
hf	-847.07	kJ/mol	Joback Method
hfus	49.63	kJ/mol	Joback Method
hvap	87.62	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	6.066		Crippen Method
mvol	345.410	ml/mol	McGowan Method
pc	1046.65	kPa	Joback Method
rinpol	2963.00		NIST Webbook
rinpol	2963.00		NIST Webbook
tb	943.60	K	Joback Method
tc	1157.33	K	Joback Method
tf	570.79	K	Joback Method
vc	1.337	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1242.28	J/molxK	943.60	Joback Method
cpg	1265.99	J/molxK	979.22	Joback Method
cpg	1289.38	J/molxK	1014.84	Joback Method
cpg	1312.63	J/molxK	1050.47	Joback Method
cpg	1335.94	J/molxK	1086.09	Joback Method
cpg	1359.49	J/molxK	1121.71	Joback Method
cpg	1383.48	J/molxK	1157.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405384&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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