Glutaric acid, 2-(adamant-1-yl)ethyl 3-methylbut-2-en-1-yl ester

Inchi: InChI=1S/C22H34O4/c1-16(2)6-8-25-20(23)4-3-5-21(24)26-9-7-22-13-17-10-18(14-22)12

InchiKey: ITYNTKDOZHEHTG-UHFFFAOYSA-N

Formula: C22H34O4

SMILES: CC(C)=CCOC(=O)CCCC(=O)OCCC12CC3CC(CC(C3)C1)C2

Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
gf	-104.86	kJ/mol	Joback Method
hf	-672.44	kJ/mol	Joback Method
hfus	44.28	kJ/mol	Joback Method
hvap	81.37	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.816		Crippen Method
mcvol	298.840	ml/mol	McGowan Method
pc	1318.48	kPa	Joback Method
rinpol	2744.00		NIST Webbook
rinpol	2744.00		NIST Webbook
tb	879.44	K	Joback Method
tc	1091.67	K	Joback Method
tf	532.94	K	Joback Method
vc	1.157	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1022.00	J/mol×K	879.44	Joback Method
cpg	1043.30	J/mol×K	914.81	Joback Method
cpg	1064.24	J/mol×K	950.18	Joback Method
cpg	1085.02	J/mol×K	985.55	Joback Method
cpg	1105.81	J/mol×K	1020.93	Joback Method
cpg	1126.81	J/mol×K	1056.30	Joback Method
cpg	1148.21	J/mol×K	1091.67	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=U405379&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

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