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

Inchi: InChI=1S/C22H36O4/c1-15(2)16(3)26-21(24)6-4-5-20(23)25-8-7-22-12-17-9-18(13-22)11

InchiKey: XLJGXZBIWNTPQA-UHFFFAOYSA-N

Formula: C22H36O4

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

Mol. weight [g/mol]: 364.52

Physical Properties

Property code	Value	Unit	Source
gf	-181.41	kJ/mol	Joback Method
hf	-790.43	kJ/mol	Joback Method
hfus	38.34	kJ/mol	Joback Method
hvap	80.55	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.894		Crippen Method
mcvol	303.140	ml/mol	McGowan Method
pc	1280.08	kPa	Joback Method
rinpol	2626.00		NIST Webbook
rinpol	2626.00		NIST Webbook
tb	874.52	K	Joback Method
tc	1084.61	K	Joback Method
tf	521.98	K	Joback Method
vc	1.163	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1049.82	J/mol×K	874.52	Joback Method
cpg	1071.47	J/mol×K	909.53	Joback Method
cpg	1092.60	J/mol×K	944.55	Joback Method
cpg	1113.39	J/mol×K	979.56	Joback Method
cpg	1133.99	J/mol×K	1014.58	Joback Method
cpg	1154.59	J/mol×K	1049.59	Joback Method
cpg	1175.35	J/mol×K	1084.61	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=U405377&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