

Glutaric acid, oct-1-en-3-yl naphth-2-ylmethyl ester

Inchi:	InChI=1S/C24H30O4/c1-3-5-6-12-22(4-2)28-24(26)14-9-13-23(25)27-18-19-15-16-20-10
InchiKey:	QMQATFFPEQDZTB-UHFFFAOYSA-N
Formula:	C24H30O4
SMILES:	C=CC(CCCCC)OC(=O)CCCC(=O)OCc1ccc2ccccc2c1
Mol. weight [g/mol]:	382.49

Physical Properties

Property code	Value	Unit	Source
gf	-21.81	kJ/mol	Joback Method
hf	-492.01	kJ/mol	Joback Method
hfus	49.36	kJ/mol	Joback Method
hvap	90.85	kJ/mol	Joback Method
log10ws	-7.29		Crippen Method
logp	5.731		Crippen Method
mcvol	316.380	ml/mol	McGowan Method
pc	1258.37	kPa	Joback Method
rinpol	2986.00		NIST Webbook
tb	947.98	K	Joback Method
tc	1166.95	K	Joback Method
tf	559.44	K	Joback Method
vc	1.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1011.18	J/molxK	947.98	Joback Method
cpg	1026.19	J/molxK	984.47	Joback Method
cpg	1040.07	J/molxK	1020.97	Joback Method
cpg	1052.89	J/molxK	1057.46	Joback Method
cpg	1064.71	J/molxK	1093.96	Joback Method
cpg	1075.63	J/molxK	1130.45	Joback Method
cpg	1085.69	J/molxK	1166.95	Joback Method
dvisc	0.0005465	Paxs	559.44	Joback Method
dvisc	0.0003154	Paxs	624.20	Joback Method

dvisc	0.0002019	Paxs	688.95	Joback Method
dvisc	0.0001395	Paxs	753.71	Joback Method
dvisc	0.0001022	Paxs	818.47	Joback Method
dvisc	0.0000784	Paxs	883.22	Joback Method
dvisc	0.0000623	Paxs	947.98	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U405359&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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