

Glutaric acid, tridec-2-yn-1-yl 3-ethylphenyl ester

Inchi:	InChI=1S/C26H38O4/c1-3-5-6-7-8-9-10-11-12-13-14-21-29-25(27)19-16-20-26(28)30-24
InchiKey:	GPENRBBZHWTLHE-UHFFFAOYSA-N
Formula:	C26H38O4
SMILES:	CCCCCCCCC#CCOC(=O)CCCC(=O)Oc1cccc(CC)c1
Mol. weight [g/mol]:	414.58

Physical Properties

Property code	Value	Unit	Source
gf	5.78	kJ/mol	Joback Method
hf	-572.21	kJ/mol	Joback Method
hfus	65.44	kJ/mol	Joback Method
hvap	96.87	kJ/mol	Joback Method
log10ws	-7.94		Crippen Method
logp	6.402		Crippen Method
mcvol	359.720	ml/mol	McGowan Method
pc	1010.37	kPa	Joback Method
rinqol	3074.00		NIST Webbook
tb	987.52	K	Joback Method
tc	1209.32	K	Joback Method
tf	672.14	K	Joback Method
vc	1.393	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1187.38	J/molxK	987.52	Joback Method
cpg	1203.66	J/molxK	1024.49	Joback Method
cpg	1218.47	J/molxK	1061.45	Joback Method
cpg	1231.84	J/molxK	1098.42	Joback Method
cpg	1243.81	J/molxK	1135.39	Joback Method
cpg	1254.45	J/molxK	1172.35	Joback Method
cpg	1263.78	J/molxK	1209.32	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=U391831&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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