

Diallyl pimelate

Inchi:	InChI=1S/C13H20O4/c1-3-10-16-12(14)8-6-5-7-9-13(15)17-11-4-2/h3-4H,1-2,5-11H2
InchiKey:	SQBBIIARQXLCHP-UHFFFAOYSA-N
Formula:	C13H20O4
SMILES:	C=CCOC(=O)CCCCC(=O)OCC=C
Mol. weight [g/mol]:	240.30

Physical Properties

Property code	Value	Unit	Source
gf	-233.58	kJ/mol	Joback Method
hf	-550.39	kJ/mol	Joback Method
hfus	32.44	kJ/mol	Joback Method
hvap	61.50	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.395		Crippen Method
mcvol	200.310	ml/mol	McGowan Method
pc	1906.90	kPa	Joback Method
rinpol	1610.00		NIST Webbook
tb	642.78	K	Joback Method
tc	824.22	K	Joback Method
tf	377.07	K	Joback Method
vc	0.773	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.47	J/mol×K	642.78	Joback Method
cpg	537.50	J/mol×K	673.02	Joback Method
cpg	550.86	J/mol×K	703.26	Joback Method
cpg	563.55	J/mol×K	733.50	Joback Method
cpg	575.59	J/mol×K	763.74	Joback Method
cpg	586.98	J/mol×K	793.98	Joback Method
cpg	597.73	J/mol×K	824.22	Joback Method
dvisc	0.0015496	Paxs	377.07	Joback Method
dvisc	0.0008532	Paxs	421.36	Joback Method

dvisc	0.0005263	Paxs	465.64	Joback Method
dvisc	0.0003530	Paxs	509.93	Joback Method
dvisc	0.0002524	Paxs	554.21	Joback Method
dvisc	0.0001897	Paxs	598.50	Joback Method
dvisc	0.0001482	Paxs	642.78	Joback Method

Sources

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=R542322&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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