Pimelic acid, butyl 1-naphthyl ester

Inchi: InChI=1S/C21H26O4/c1-2-3-16-24-20(22)14-5-4-6-15-21(23)25-19-13-9-11-17-10-7-8-12
InchiKey: FPBRBPLOTRADHE-UHFFFAOYSA-N
Formula: C21H26O4
SMILES: CCCCOC(=O)CCCCCC(=O)Oc1cccc2ccccc12
Mol. weight [g/mol]: 342.43

Physical Properties

Property code	Value	Unit	Source
gf	-132.47	kJ/mol	Joback Method
hf	-550.24	kJ/mol	Joback Method
hfus	46.39	kJ/mol	Joback Method
hvap	85.23	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	5.039		Crippen Method
mcvol	278.410	ml/mol	McGowan Method
pc	1501.15	kPa	Joback Method
rinpol	2738.00		NIST Webbook
tb	883.10	K	Joback Method
tc	1096.62	K	Joback Method
tf	542.39	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	861.05	J/mol×K	883.10	Joback Method
cpg	924.33	J/mol×K	1061.03	Joback Method
cpg	913.64	J/mol×K	1025.45	Joback Method
cpg	902.02	J/mol×K	989.86	Joback Method
cpg	889.42	J/mol×K	954.27	Joback Method
cpg	875.78	J/mol×K	918.69	Joback Method
cpg	934.15	J/mol×K	1096.62	Joback Method
dvisc	0.0000952	Pa×s	883.10	Joback Method
dvisc	0.0001176	Pa×s	826.31	Joback Method

dvisc	0.0001497	Pa×s	769.53	Joback Method
dvisc	0.0001982	Pa×s	712.74	Joback Method
dvisc	0.0002754	Pa×s	655.96	Joback Method
dvisc	0.0004074	Pa×s	599.17	Joback Method
dvisc	0.0006540	Pa×s	542.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416719&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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