

Fumaric acid, naphth-2-yl dodec-2-en-1-yl ester

Inchi: InChI=1S/C26H32O4/c1-2-3-4-5-6-7-8-9-10-13-20-29-25(27)18-19-26(28)30-24-17-16-22
InchiKey: BKKPMNKCICKSJSV-FOYOAPBKSA-N
Formula: C26H32O4
SMILES: CCCCCCCCCC=CCOC(=O)C=CC(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]: 408.53

Physical Properties

Property code	Value	Unit	Source
gf	70.07	kJ/mol	Joback Method
hf	-419.00	kJ/mol	Joback Method
hfus	59.74	kJ/mol	Joback Method
hvap	96.28	kJ/mol	Joback Method
log10ws	-8.02		Crippen Method
logp	6.541		Crippen Method
mcvol	340.260	ml/mol	McGowan Method
pc	1143.66	kPa	Joback Method
rinpol	3211.00		NIST Webbook
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tb	1005.82	K	Joback Method
tc	1233.45	K	Joback Method
tf	588.58	K	Joback Method
vc	1.313	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1104.72	J/mol×K	1005.82	Joback Method
cpg	1175.37	J/mol×K	1195.51	Joback Method
cpg	1162.59	J/mol×K	1157.57	Joback Method
cpg	1149.25	J/mol×K	1119.64	Joback Method
cpg	1135.23	J/mol×K	1081.70	Joback Method
cpg	1120.42	J/mol×K	1043.76	Joback Method
cpg	1187.71	J/mol×K	1233.45	Joback Method
dvisc	0.0000370	Pa×s	1005.82	Joback Method

dvisc	0.0000467	Pa×s	936.28	Joback Method
dvisc	0.0000611	Pa×s	866.74	Joback Method
dvisc	0.0000837	Pa×s	797.20	Joback Method
dvisc	0.0001218	Pa×s	727.66	Joback Method
dvisc	0.0001920	Pa×s	658.12	Joback Method
dvisc	0.0003369	Pa×s	588.58	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=U405837&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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