

Fumaric acid, 2-pentyl naphth-2-ylmethyl ester

Inchi: InChI=1S/C20H22O4/c1-3-6-15(2)24-20(22)12-11-19(21)23-14-16-9-10-17-7-4-5-8-18(17)
InchiKey: TVVDUBSOBJONGT-VAWYXSNFSA-N
Formula: C20H22O4
SMILES: CCCC(C)OC(=O)C=CC(=O)OCc1ccc2ccccc2c1
Mol. weight [g/mol]: 326.39

Physical Properties

Property code	Value	Unit	Source
gf	-63.11	kJ/mol	Joback Method
hf	-417.66	kJ/mol	Joback Method
hfus	40.48	kJ/mol	Joback Method
hvap	82.57	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	4.171		Crippen Method
mvol	260.020	ml/mol	McGowan Method
pc	1700.50	kPa	Joback Method
rinpol	2590.00		NIST Webbook
rinpol	2590.00		NIST Webbook
tb	863.94	K	Joback Method
tc	1085.85	K	Joback Method
tf	511.04	K	Joback Method
vc	0.992	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	776.26	J/molxK	863.94	Joback Method
cpg	790.51	J/molxK	900.92	Joback Method
cpg	803.73	J/molxK	937.91	Joback Method
cpg	815.99	J/molxK	974.89	Joback Method
cpg	827.35	J/molxK	1011.88	Joback Method
cpg	837.89	J/molxK	1048.86	Joback Method
cpg	847.67	J/molxK	1085.85	Joback Method
dvisc	0.0007089	Paxs	511.04	Joback Method

dvisc	0.0004169	Paxs	569.86	Joback Method
dvisc	0.0002708	Paxs	628.67	Joback Method
dvisc	0.0001893	Paxs	687.49	Joback Method
dvisc	0.0001401	Paxs	746.31	Joback Method
dvisc	0.0001083	Paxs	805.12	Joback Method
dvisc	0.0000867	Paxs	863.94	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=U405568&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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